

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN120320\
 Data File : VN064896.D
 Acq On : 3 Dec 2020 13:47
 Operator : JC/MD
 Sample : L4918-01
 Misc : 5.08g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 20801

Integration Parameters: RTEINT.P

Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N112320W.M
 Title : SW846 8260

Signal : TIC: VN064895.D

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.782	609	635	708	rBV	7447581	26896074	76.63%	15.178%
2	7.582	1787	1817	1838	rBV3	1518408	4611700	13.14%	2.602%
3	7.695	1839	1852	1872	rVB2	487810	1271093	3.62%	0.717%
4	7.827	1873	1893	1925	rBV	2166112	5270196	15.01%	2.974%
5	7.984	1926	1942	1962	rBV3	143995	375100	1.07%	0.212%
6	8.106	1962	1980	1990	rBV4	331341	841247	2.40%	0.475%
7	8.393	2047	2069	2096	rBV	2647893	5461083	15.56%	3.082%
8	8.544	2101	2116	2141	rVV	338221	743472	2.12%	0.420%
9	9.042	2242	2271	2282	rBV3	621787	1621528	4.62%	0.915%
10	9.103	2282	2290	2303	rVB	190162	369639	1.05%	0.209%
11	9.479	2387	2407	2428	rBV3	177068	382896	1.09%	0.216%
12	9.621	2428	2451	2462	rBV4	220870	580683	1.65%	0.328%
13	9.692	2463	2473	2497	rVB2	315999	798550	2.28%	0.451%
14	9.833	2497	2517	2539	rBV	275338	687538	1.96%	0.388%
15	10.055	2574	2586	2594	rVV3	652371	1266093	3.61%	0.714%
16	10.122	2594	2607	2631	rVV	16539982	35099824	100.00%	19.807%
17	10.251	2633	2647	2659	rVB	579366	1118971	3.19%	0.631%
18	10.975	2862	2872	2883	rVB2	248073	441913	1.26%	0.249%
19	11.171	2916	2933	2952	rVB5	548754	1293462	3.69%	0.730%
20	11.270	2952	2964	2986	rBV	484236	905931	2.58%	0.511%
21	11.376	2987	2997	3016	rBV	506464	935827	2.67%	0.528%
22	11.483	3017	3030	3045	rBV	746158	1398034	3.98%	0.789%
23	11.598	3045	3066	3082	rVV2	3116370	7810680	22.25%	4.408%
24	11.920	3145	3166	3180	rBV2	1287758	3015163	8.59%	1.701%
25	12.016	3188	3196	3210	rVB	802467	1178799	3.36%	0.665%
26	12.093	3211	3220	3224	rBV4	472258	764043	2.18%	0.431%
27	12.132	3225	3232	3250	rVB5	911239	1700716	4.85%	0.960%
28	12.219	3252	3259	3265	rBV3	275837	422880	1.20%	0.239%
29	12.309	3281	3287	3292	rBV	506972	627473	1.79%	0.354%
30	12.376	3302	3308	3315	rVB	343397	453193	1.29%	0.256%
31	12.418	3315	3321	3330	rVB	528736	686784	1.96%	0.388%
32	12.534	3349	3357	3361	rBV3	515018	795390	2.27%	0.449%
33	12.563	3362	3366	3374	rVB	714671	901092	2.57%	0.508%
34	12.627	3374	3386	3393	rBV	2574028	4397832	12.53%	2.482%

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35	12.701	3401	3409	3420	rVB2	4983807	7866034	22.41%	4.439%
36	12.804	3431	3441	3450	rBV	4261143	6454277	18.39%	3.642%
37	12.865	3452	3460	3473	rVB	977574	1646856	4.69%	0.929%
38	12.936	3475	3482	3494	rVB	847733	1384076	3.94%	0.781%
39	13.013	3495	3506	3514	rBV	4954812	8219844	23.42%	4.638%
40	13.142	3533	3546	3554	rVB4	467654	1042153	2.97%	0.588%
41	13.216	3555	3569	3581	rBV5	1153472	3659466	10.43%	2.065%
42	13.347	3596	3610	3620	rVB2	1621197	3460178	9.86%	1.953%
43	13.515	3647	3662	3669	rBV	1572876	2883166	8.21%	1.627%
44	13.560	3669	3676	3692	rVB4	1252465	2654273	7.56%	1.498%
45	13.643	3692	3702	3711	rBV3	1482774	2365052	6.74%	1.335%
46	13.714	3718	3724	3733	rVB	479867	715600	2.04%	0.404%
47	13.775	3735	3743	3747	rVV	607105	912721	2.60%	0.515%
48	13.804	3748	3752	3761	rVB	705607	951125	2.71%	0.537%
49	13.862	3762	3770	3779	rVB	1022835	1572552	4.48%	0.887%
50	13.968	3793	3803	3813	rVB	952851	1576793	4.49%	0.890%
51	14.100	3836	3844	3850	rBV2	265960	415187	1.18%	0.234%
52	14.219	3875	3881	3889	rVB	726845	1070108	3.05%	0.604%
53	14.267	3889	3896	3903	rBV3	382182	525727	1.50%	0.297%
54	14.306	3903	3908	3921	rVB3	284983	402074	1.15%	0.227%
55	14.447	3945	3952	3961	rVV4	418669	794590	2.26%	0.448%
56	14.495	3962	3967	3975	rVB	526781	734064	2.09%	0.414%
57	14.556	3975	3986	3999	rBV5	1038399	2299735	6.55%	1.298%
58	14.621	4000	4006	4016	rVB	251532	396820	1.13%	0.224%
59	14.823	4061	4069	4076	rBV3	331368	563277	1.60%	0.318%
60	14.929	4092	4102	4114	rVB3	361358	749894	2.14%	0.423%
61	15.100	4139	4155	4167	rVB	537724	1148447	3.27%	0.648%
62	15.209	4180	4189	4197	rBV3	297030	506750	1.44%	0.286%
63	15.299	4210	4217	4231	rVB5	251250	475093	1.35%	0.268%
64	15.383	4232	4243	4256	rBV2	361770	661331	1.88%	0.373%
65	15.540	4276	4292	4299	rBV5	199192	558244	1.59%	0.315%
66	15.730	4341	4351	4362	rBV4	195431	414246	1.18%	0.234%
67	16.116	4461	4471	4485	rVB	961318	1831400	5.22%	1.033%
68	16.305	4518	4530	4557	rVB	514313	1173872	3.34%	0.662%

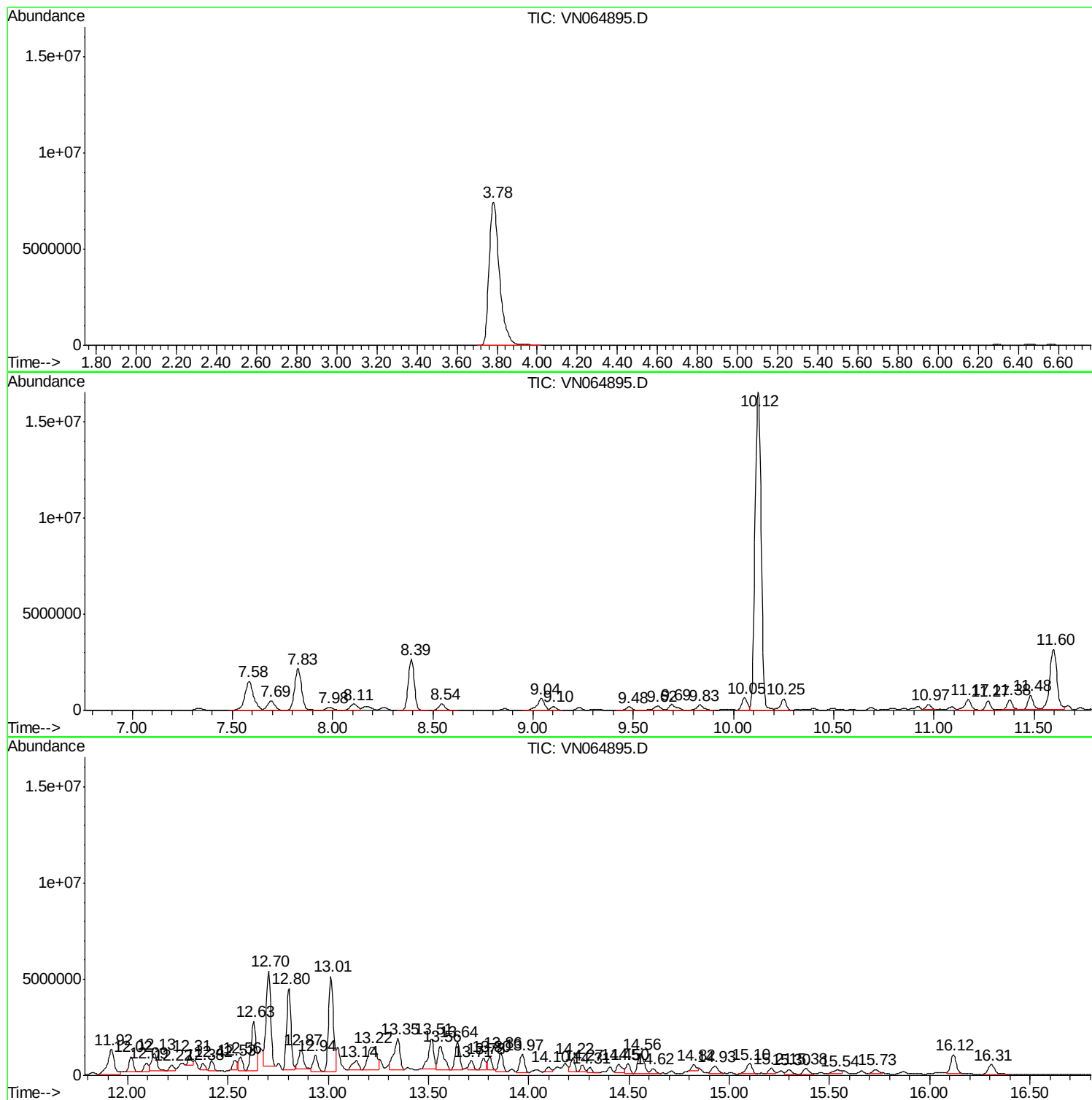
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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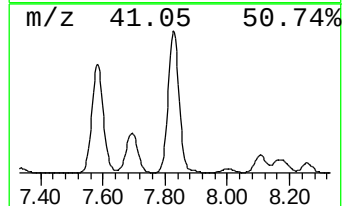
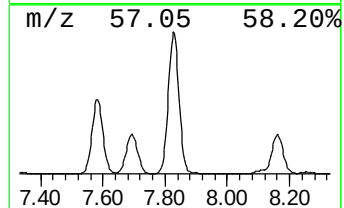
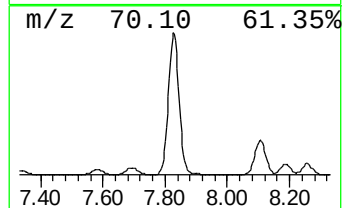
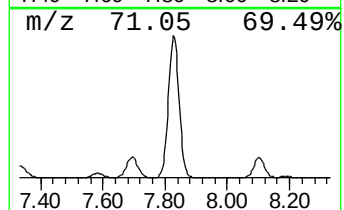
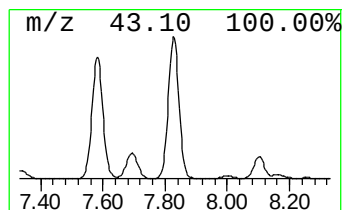
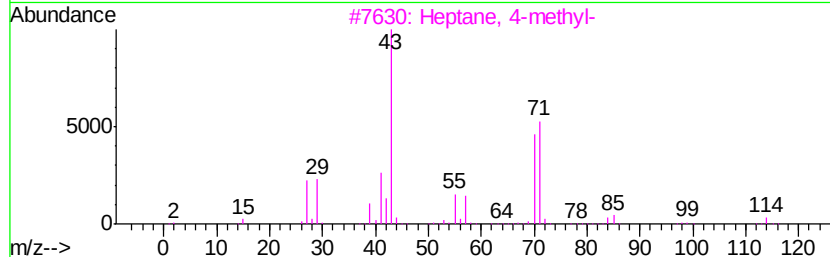
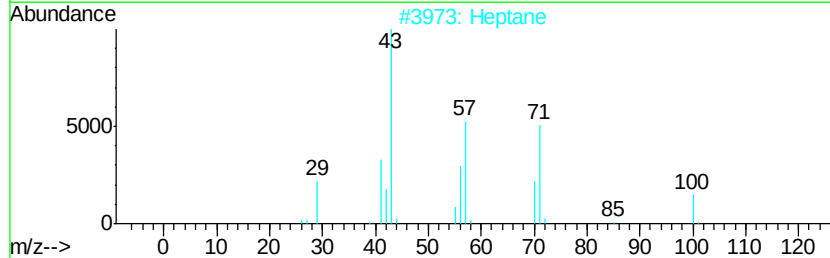
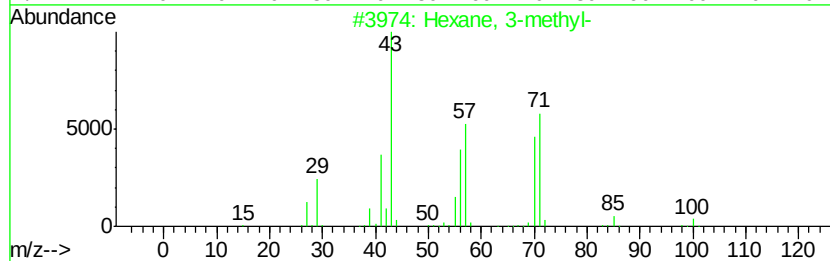
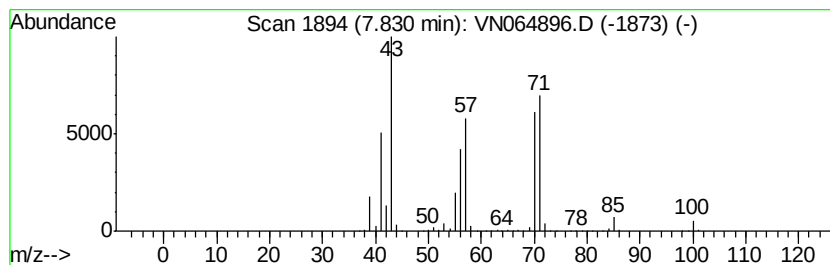
Instrument :
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ClientSampleID :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N112320W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Hexane, 3-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.		
7.83	57.14 ug/l	5270200	Pentafluorobenzene	7.62		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 3-methyl-		100	C7H16	000589-34-4	94
2	Heptane		100	C7H16	000142-82-5	80
3	Heptane, 4-methyl-		114	C8H18	000589-53-7	59
4	Pentane, 2,3,4-trimethyl-		114	C8H18	000565-75-3	53
5	Pentane, 3-ethyl-		100	C7H16	000617-78-7	53



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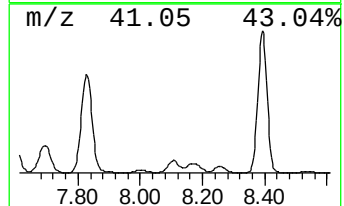
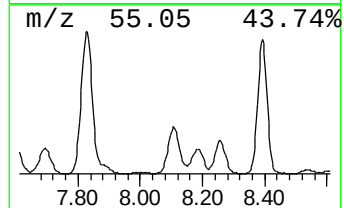
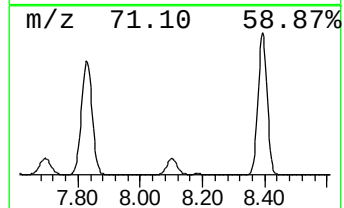
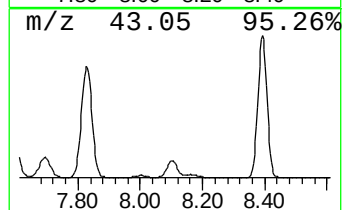
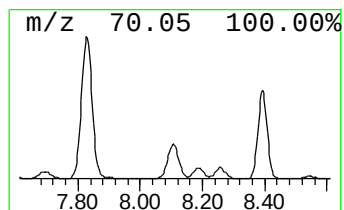
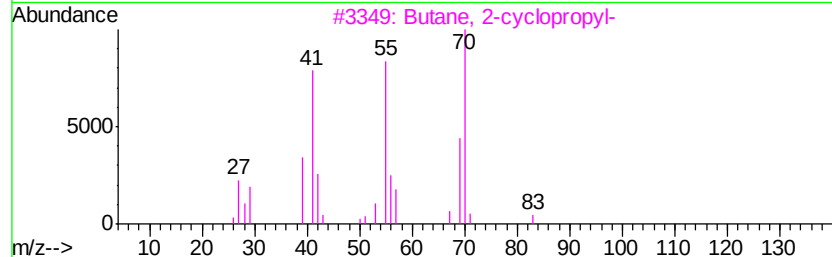
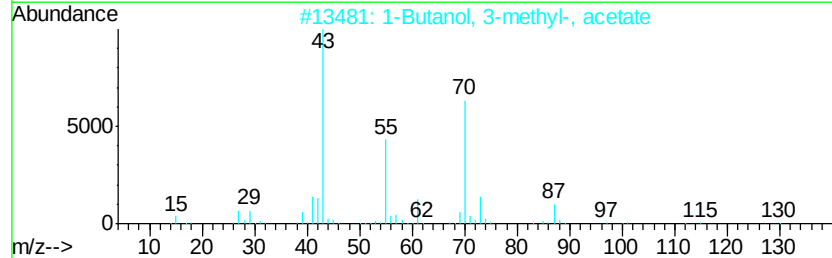
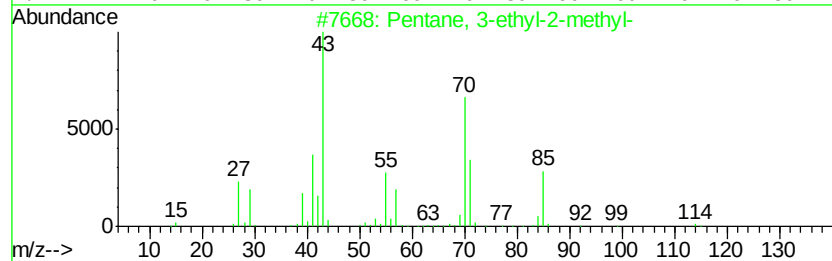
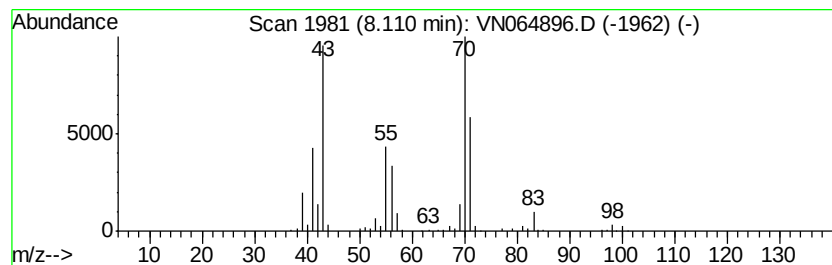
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Pentane, 3-ethyl-2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.11	56.58 ug/l	841247	1,4-Difluorobenzene	8.54

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 3-ethyl-2-methyl-	114	C8H18	000609-26-7	72
2		1-Butanol, 3-methyl-, acetate	130	C7H14O2	000123-92-2	50
3		Butane, 2-cyclopropyl-	98	C7H14	005750-02-7	47
4		Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	45
5		Hexane, 3-methyl-	100	C7H16	000589-34-4	43



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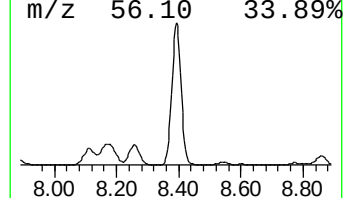
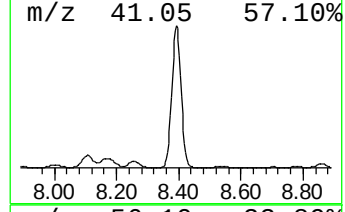
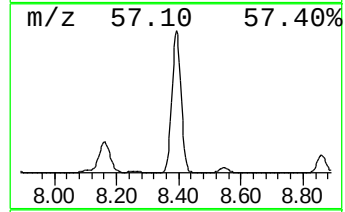
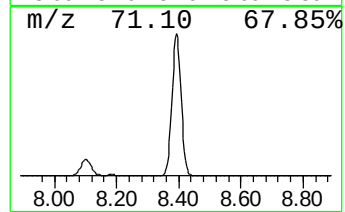
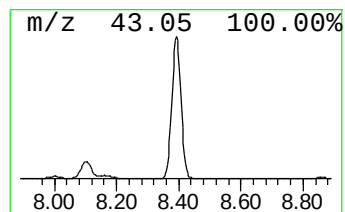
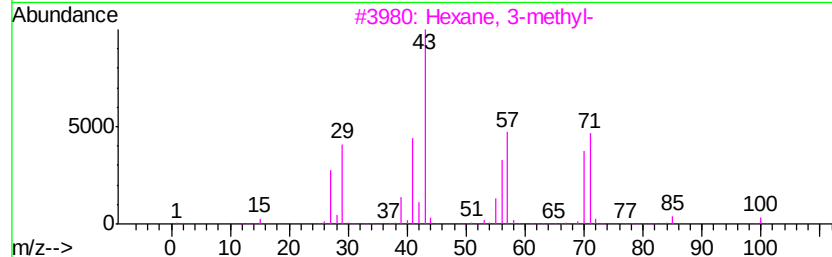
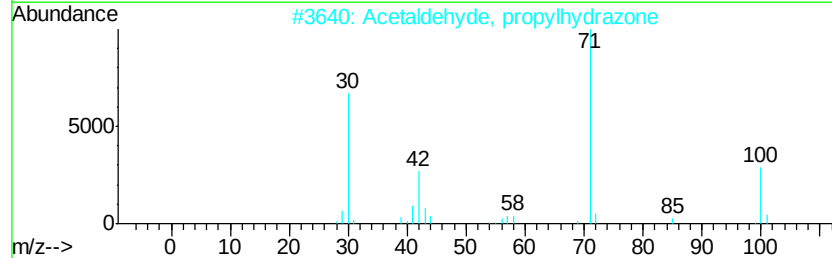
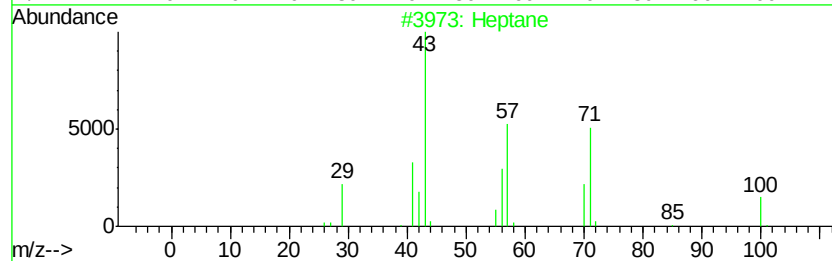
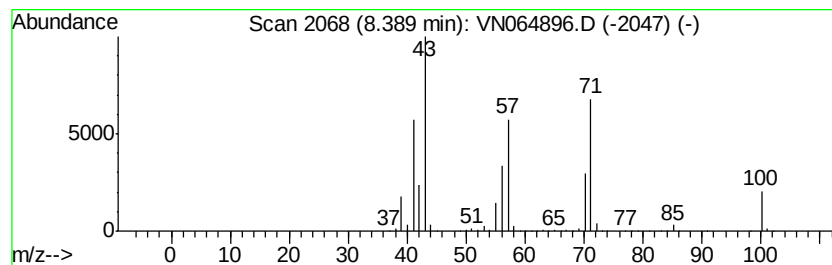
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Peak Number 3 Heptane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.39	367.27 ug/l	5461080	1,4-Difluorobenzene	8.54

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptane	100	C7H16	000142-82-5	91
2		Acetaldehyde, propylhydrazone	100	C5H12N2	007422-88-0	49
3		Hexane, 3-methyl-	100	C7H16	000589-34-4	47
4		Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	40
5		Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	37



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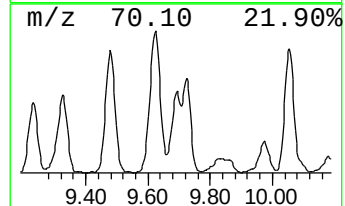
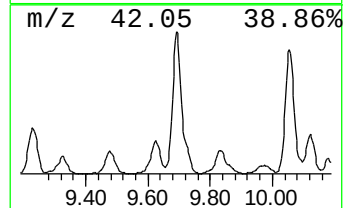
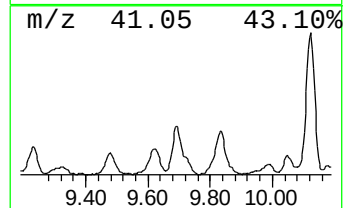
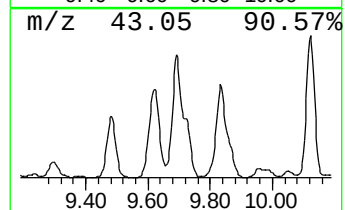
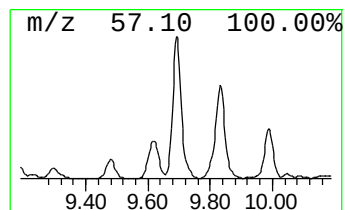
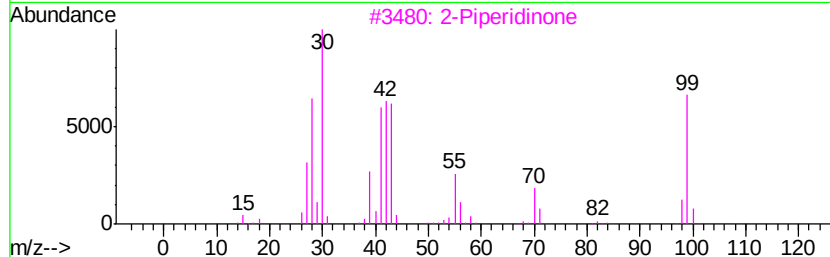
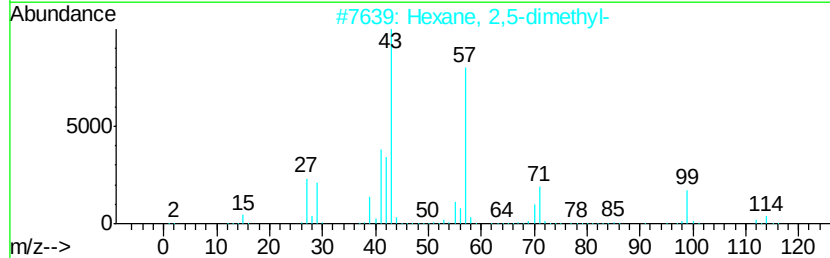
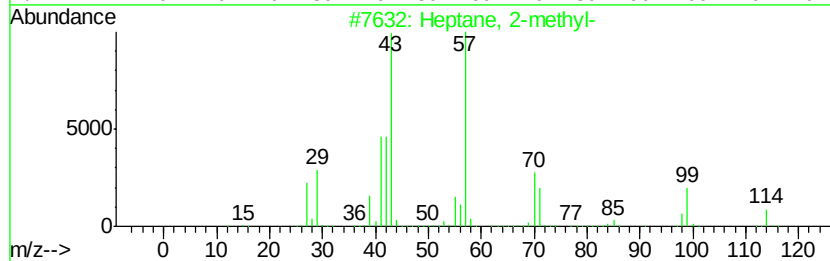
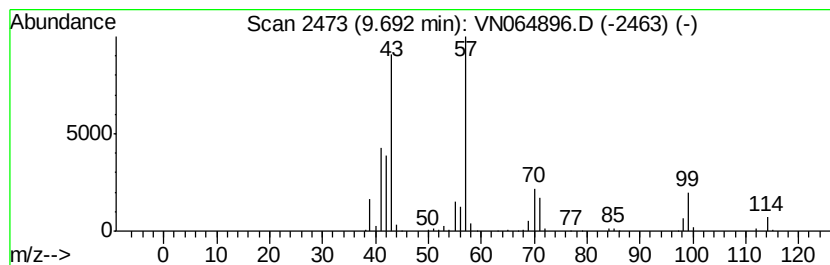
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Peak Number 4 Heptane, 2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.69	53.70 ug/l	798550	1,4-Difluorobenzene	8.54

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptane, 2-methyl-	114	C8H18	000592-27-8	94
2		Hexane, 2,5-dimethyl-	114	C8H18	000592-13-2	72
3		2-Piperidinone	99	C5H9NO	000675-20-7	58
4		Pentane	72	C5H12	000109-66-0	38
5		Heptane, 2,3,6-trimethyl-	142	C10H22	004032-93-3	38



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_N\DATA\VN120320\
Data File : VN064896.D
Acq On : 3 Dec 2020 13:47
Operator : JC/MD
Sample : L4918-01
Misc : 5.08g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
20801

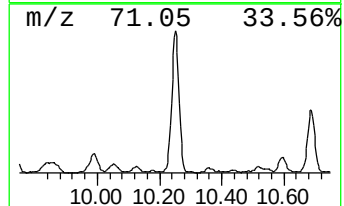
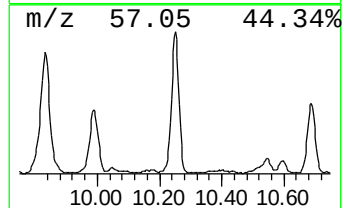
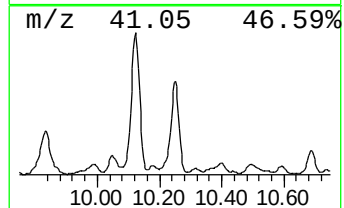
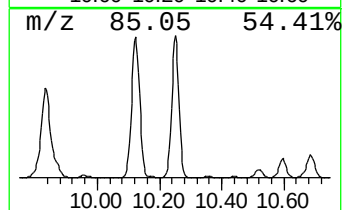
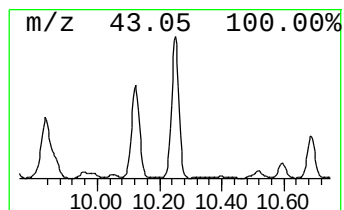
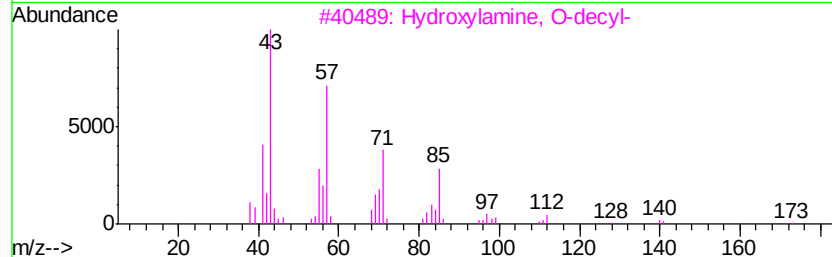
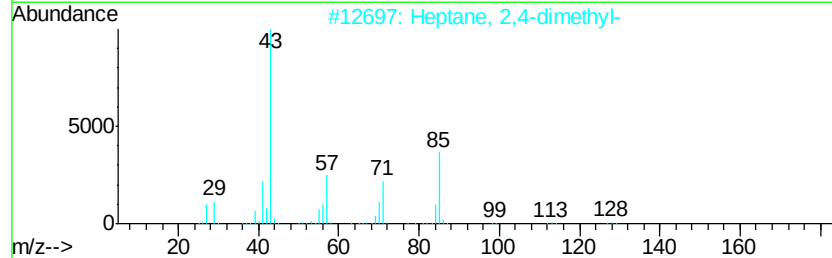
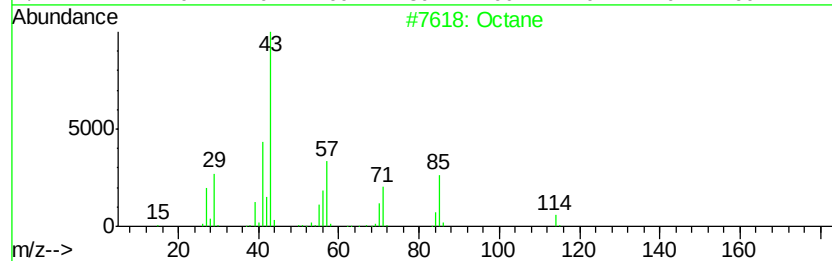
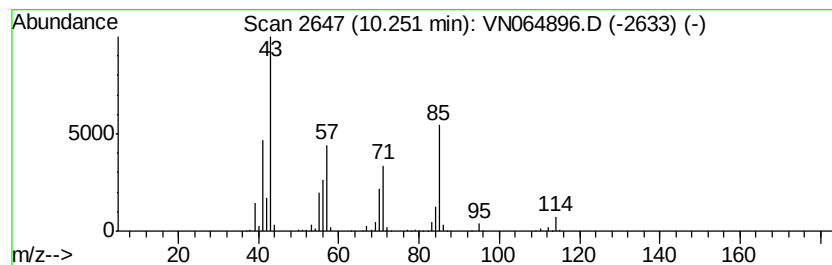
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.25	59.79 ug/l	1118970	Chlorobenzene-d5	11.38

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane		114	C8H18	000111-65-9	94
2	Heptane, 2,4-dimethyl-		128	C9H20	002213-23-2	72
3	Hydroxylamine, O-decyl-		173	C10H23NO	029812-79-1	64
4	Oxalic acid, isohexyl pentyl ester		244	C13H24O4	1000309-32-8	64
5	Hexane, 2,4-dimethyl-		114	C8H18	000589-43-5	53



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN120320\
Data File : VN064896.D
Acq On : 3 Dec 2020 13:47
Operator : JC/MD
Sample : L4918-01
Misc : 5.08g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampled :
20801

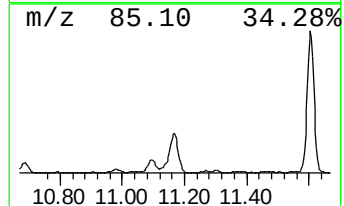
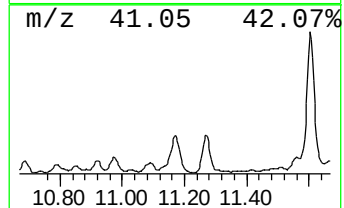
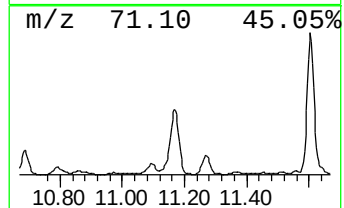
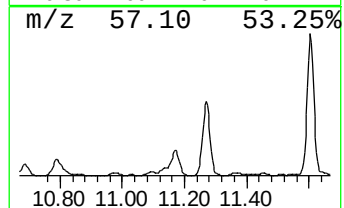
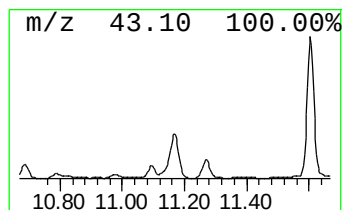
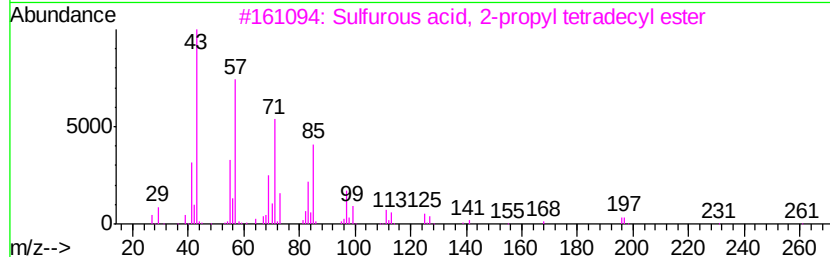
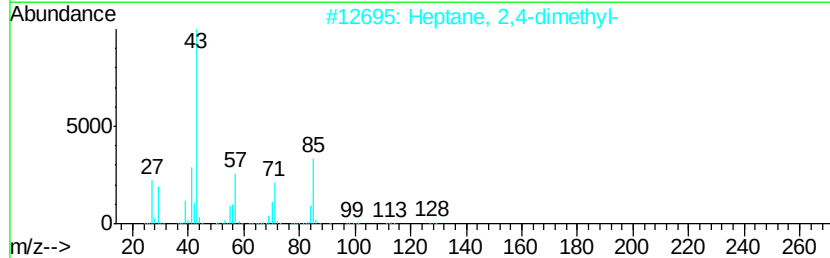
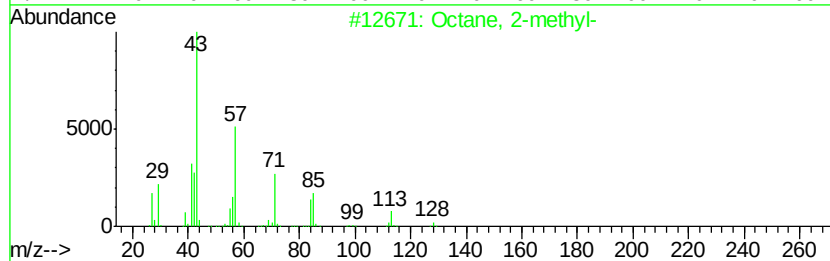
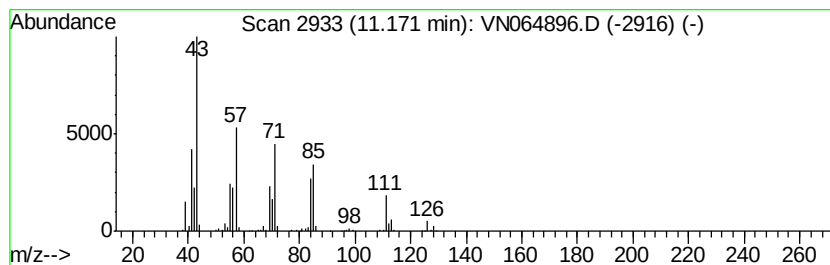
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Octane, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.17	69.11 ug/l	1293460	Chlorobenzene-d5	11.38

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octane, 2-methyl-	128	C9H20	003221-61-2	72
2		Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	52
3		Sulfurous acid, 2-propyl tetradecyl...	320	C17H36O3S	1000309-12-5	50
4		Octane, 4-methyl-	128	C9H20	002216-34-4	47
5		Octane, 3-ethyl-2,7-dimethyl-	170	C12H26	062183-55-5	47



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_N\DATA\VN120320\
Data File : VN064896.D
Acq On : 3 Dec 2020 13:47
Operator : JC/MD
Sample : L4918-01
Misc : 5.08g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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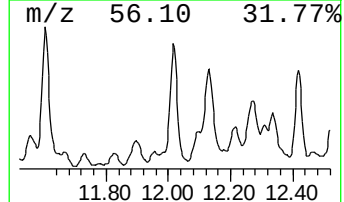
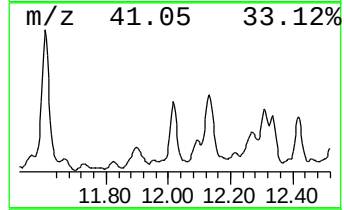
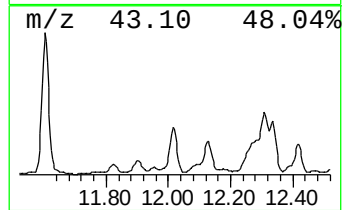
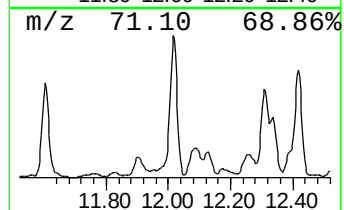
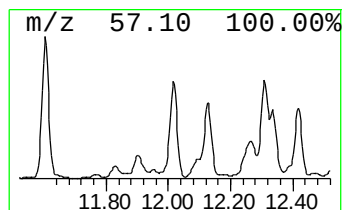
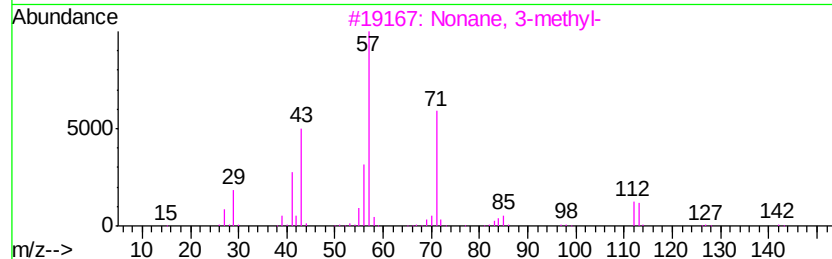
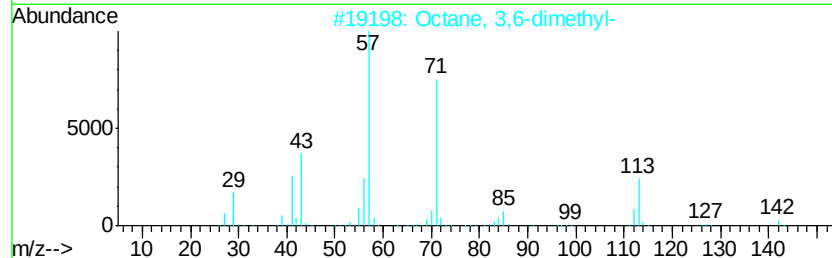
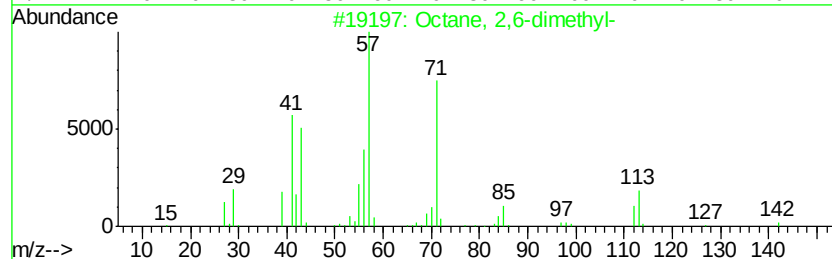
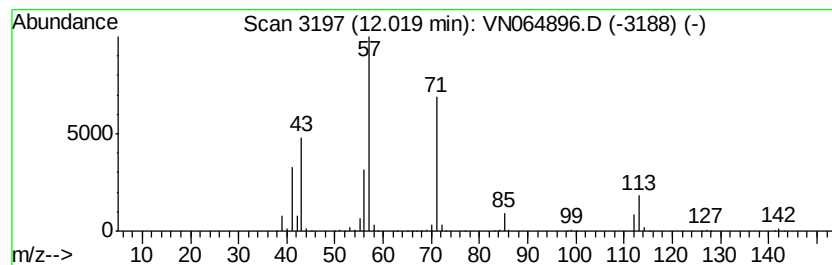
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Octane, 2,6-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.02	62.98 ug/l	1178800	Chlorobenzene-d5	11.38

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	91
2		Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	91
3		Nonane, 3-methyl-	142	C10H22	005911-04-6	87
4		Sulfurous acid, 2-ethylhexyl hex...	418	C24H50O3S	1000309-19-9	64
5		Undecane, 6,6-dimethyl-	184	C13H28	017312-76-4	64



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_N\DATA\VN120320\
Data File : VN064896.D
Acq On : 3 Dec 2020 13:47
Operator : JC/MD
Sample : L4918-01
Misc : 5.08g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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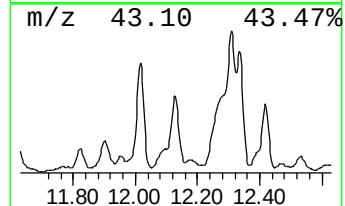
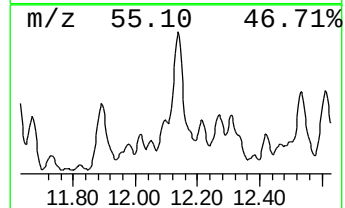
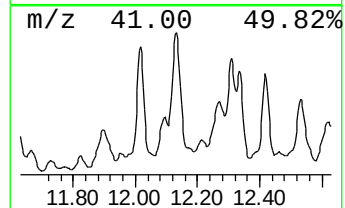
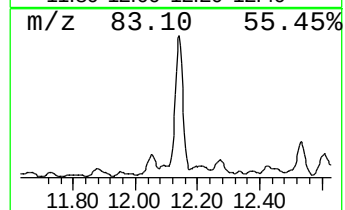
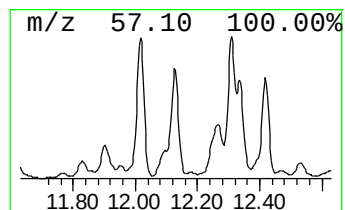
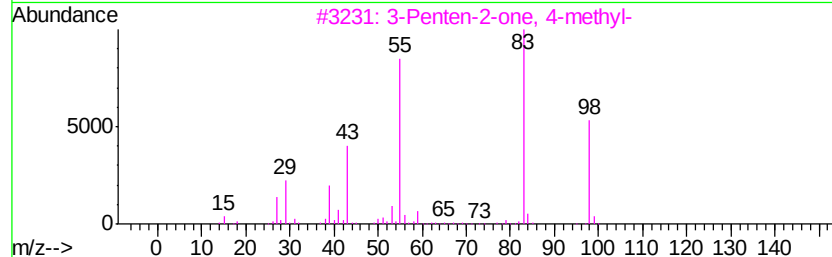
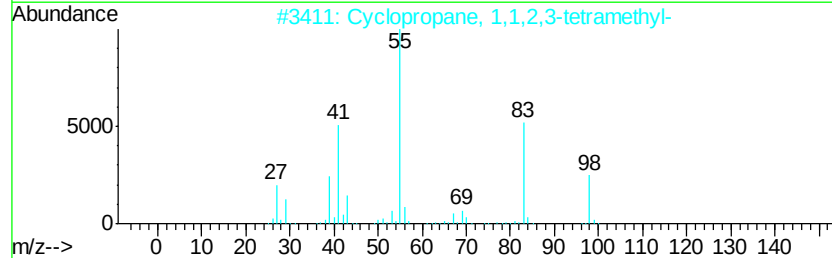
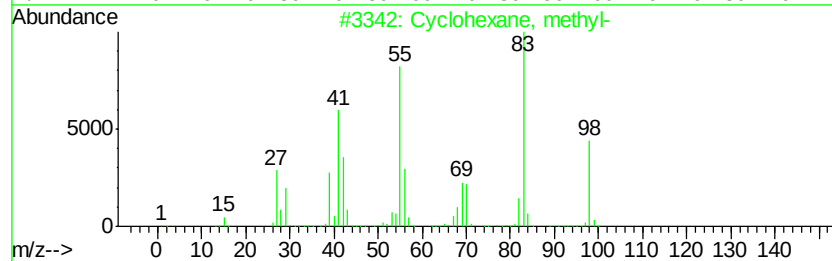
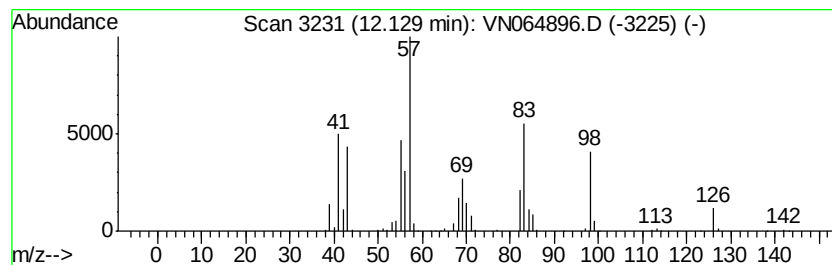
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 unknown12.13 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.13	90.87 ug/l	1700720	Chlorobenzene-d5	11.38

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, methyl-	98	C7H14	000108-87-2	53
2		Cyclopropane, 1,1,2,3-tetramethyl-	98	C7H14	074752-93-5	43
3		3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	43
4		Ethanone, 1-(1-methylcyclopentyl)-	126	C8H14O	013388-93-7	43
5		Ethanone, 1-cyclohexyl-	126	C8H14O	000823-76-7	43



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA N\DATA\VN120320\
Data File : VN064896.D
Acq On : 3 Dec 2020 13:47
Operator : JC/MD
Sample : L4918-01
Misc : 5.08g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

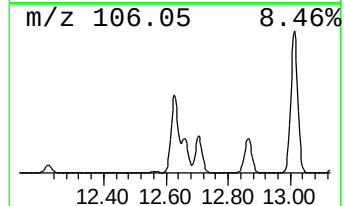
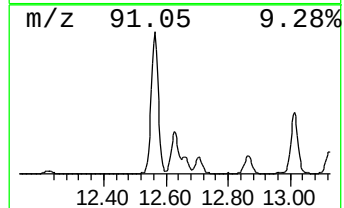
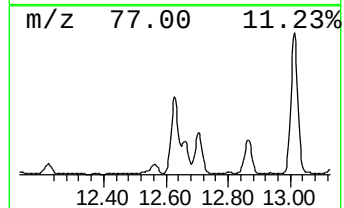
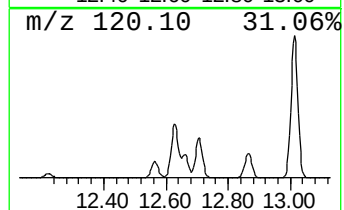
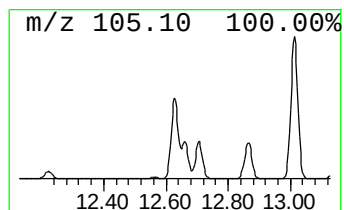
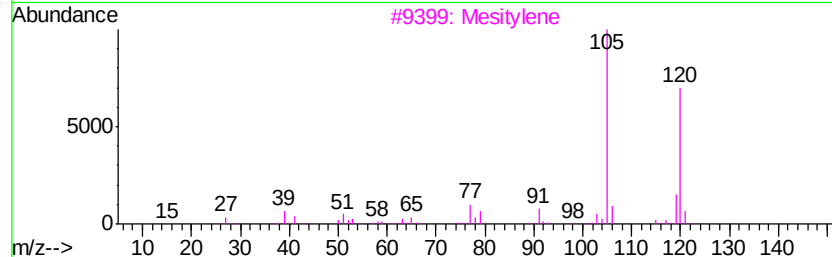
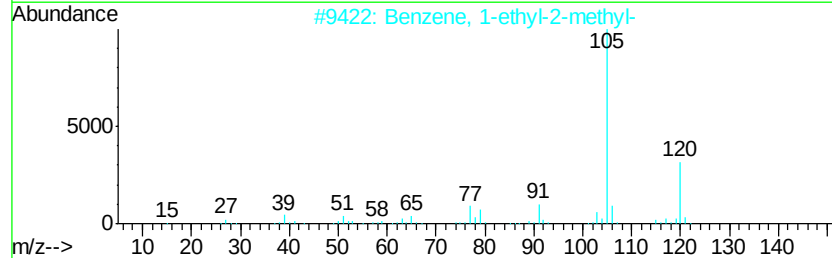
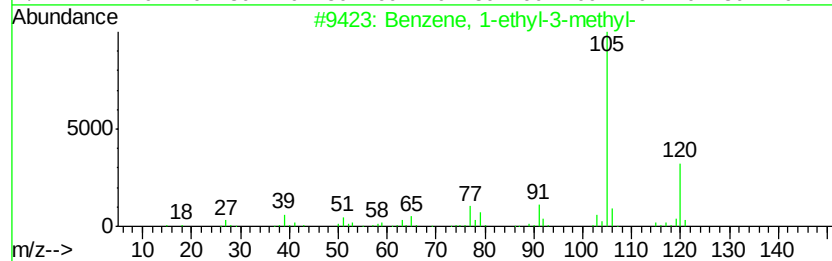
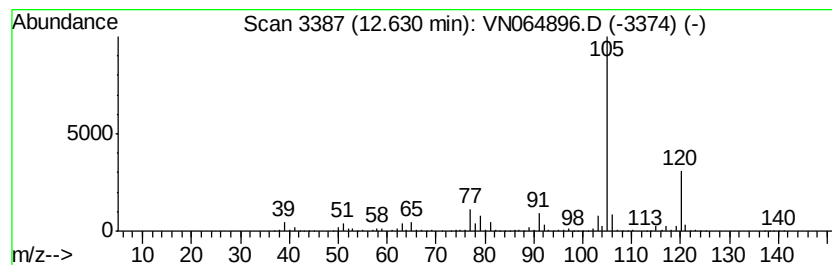
Instrument :
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ClientSampleId :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N112320W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Benzene, 1-ethyl-3-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.63	63.55 ug/l	4397830	1,4-Dichlorobenzene-d4	13.32
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzene, 1-ethyl-3-methyl-	120 C9H12	000620-14-4 95
2		Benzene, 1-ethyl-2-methyl-	120 C9H12	000611-14-3 95
3		Mesitylene	120 C9H12	000108-67-8 91
4		Benzene, 1-ethyl-4-methyl-	120 C9H12	000622-96-8 91
5		Benzene, 1,2,4-trimethyl-	120 C9H12	000095-63-6 91



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_N\DATA\VN120320\
Data File : VN064896.D
Acq On : 3 Dec 2020 13:47
Operator : JC/MD
Sample : L4918-01
Misc : 5.08g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

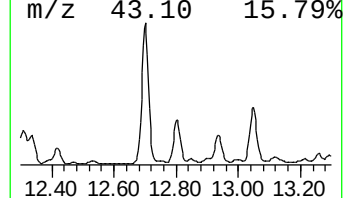
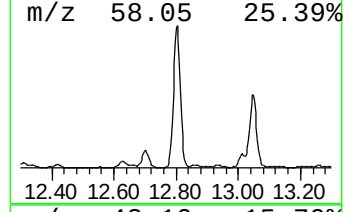
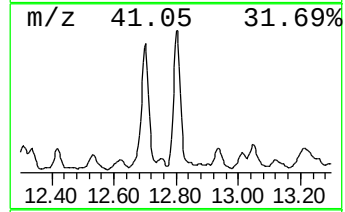
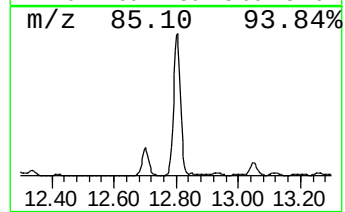
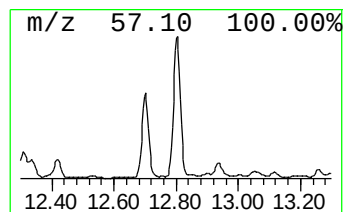
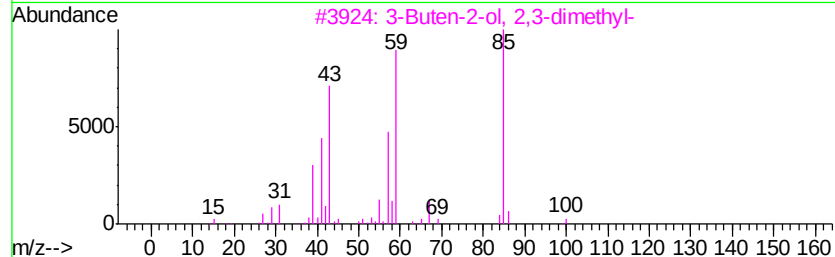
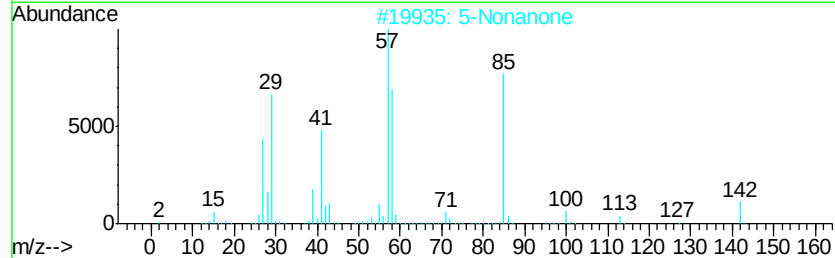
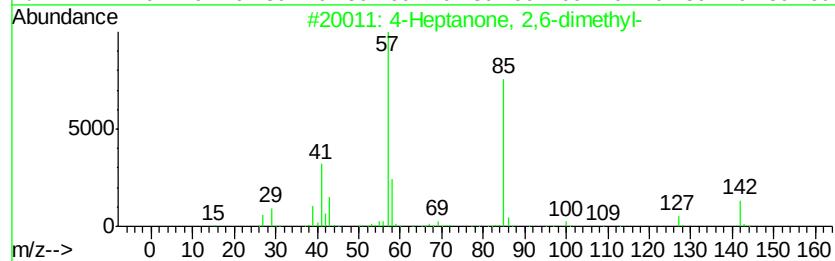
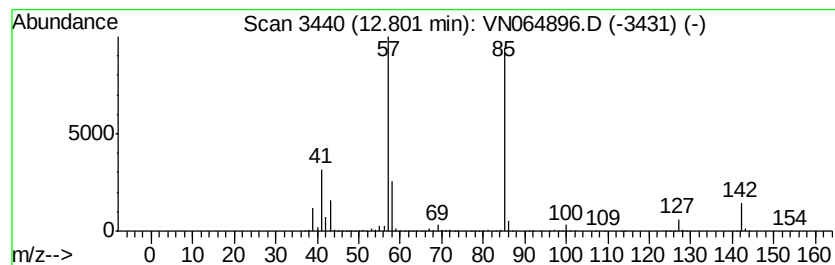
Instrument :
MSVOA_N
ClientSampled :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N112320W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 4-Heptanone, 2,6-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.80	93.27 ug/l	6454280	1,4-Dichlorobenzene-d4	13.32	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptanone, 2,6-dimethyl-	142	C9H18O	000108-83-8	94
2	5-Nonanone	142	C9H18O	000502-56-7	59
3	3-Buten-2-ol, 2,3-dimethyl-	100	C6H12O	010473-13-9	50
4	4-Octanone, 2-methyl-	142	C9H18O	007492-38-8	50
5	2-Methylbutanoic anhydride	186	C10H18O3	001468-39-9	45



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN120320\
 Data File : VN064896.D
 Acq On : 3 Dec 2020 13:47
 Operator : JC/MD
 Sample : L4918-01
 Misc : 5.08g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 20801

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N112320W.M
 Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Hexane, 3-methyl-	7.83	57.1	ug/l	5270200	1	7.62	4611700	50.0
Pentane, 3-ethyl-...	8.11	56.6	ug/l	841247	2	8.54	743472	50.0
Heptane	8.39	367.3	ug/l	5461080	2	8.54	743472	50.0
Heptane, 2-methyl-	9.69	53.7	ug/l	798550	2	8.54	743472	50.0
Octane	10.25	59.8	ug/l	1118970	3	11.38	935827	50.0
Octane, 2-methyl-	11.17	69.1	ug/l	1293460	3	11.38	935827	50.0
Octane, 2,6-dimet...	12.02	63.0	ug/l	1178800	3	11.38	935827	50.0
unknown12.13	12.13	90.9	ug/l	1700720	3	11.38	935827	50.0
Benzene, 1-ethyl-...	12.63	63.5	ug/l	4397830	4	13.32	3460180	50.0
4-Heptanone, 2,6-...	12.80	93.3	ug/l	6454280	4	13.32	3460180	50.0