

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN112119\
 Data File : VN059343.D
 Acq On : 21 Nov 2019 18:02
 Operator : JC/SP
 Sample : K5957-12
 Misc : 5.52g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-5-(16-18)

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\82N112019W.M
 Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	7.641	1813	1825	1841	rVB	448015	1094725	1.16%	0.089%
2	8.567	2096	2113	2137	rBV	637649	1323283	1.41%	0.107%
3	9.066	2243	2268	2280	rBV2	413367	990790	1.05%	0.080%
4	9.719	2459	2471	2493	rVB2	760678	1868705	1.99%	0.151%
5	9.857	2493	2514	2537	rVB	651263	1612661	1.72%	0.131%
6	10.079	2569	2583	2593	rBV3	2174254	4517073	4.81%	0.366%
7	10.249	2628	2636	2658	rVB4	391678	1157923	1.23%	0.094%
8	10.426	2682	2691	2707	rVB	1146027	2169640	2.31%	0.176%
9	10.522	2708	2721	2730	rBV3	620970	1326726	1.41%	0.107%
10	10.622	2743	2752	2761	rVB	675406	1071967	1.14%	0.087%
11	10.715	2770	2781	2792	rVB	2550881	4307595	4.58%	0.349%
12	10.815	2799	2812	2824	rBV	1526620	3201394	3.41%	0.259%
13	10.882	2825	2833	2840	rBV4	1025039	1767805	1.88%	0.143%
14	10.947	2844	2853	2861	rBV	3628739	5592906	5.95%	0.453%
15	11.001	2861	2870	2881	rVB2	6487173	11344825	12.07%	0.918%
16	11.056	2881	2887	2894	rVB	974884	1336477	1.42%	0.108%
17	11.120	2894	2907	2915	rBV5	4013931	7669441	8.16%	0.621%
18	11.198	2915	2931	2950	rVB6	6958086	20346966	21.65%	1.647%
19	11.300	2950	2963	2985	rBV	8809125	18074019	19.23%	1.463%
20	11.400	2986	2994	3001	rBV2	841010	1492612	1.59%	0.121%
21	11.509	3015	3028	3033	rBV2	3856839	7608413	8.10%	0.616%
22	11.542	3034	3038	3044	rVB	2696432	3185727	3.39%	0.258%
23	11.593	3045	3054	3063	rBV6	5521574	11147953	11.86%	0.903%
24	11.657	3064	3074	3081	rBV3	11717093	23186811	24.67%	1.877%
25	11.696	3082	3086	3097	rVB3	10526194	16604768	17.67%	1.344%
26	11.760	3097	3106	3112	rBV3	2608378	4743719	5.05%	0.384%
27	11.812	3114	3122	3128	rBV2	1672288	2777841	2.96%	0.225%
28	11.853	3128	3135	3143	rBV3	4493187	6519198	6.94%	0.528%
29	11.927	3143	3158	3171	rBV7	17830415	53747644	57.19%	4.351%
30	12.050	3188	3196	3204	rBV	14697463	25149960	26.76%	2.036%
31	12.124	3211	3219	3224	rBV4	15680631	25893416	27.55%	2.096%
32	12.165	3225	3232	3250	rVB6	23875448	50177584	53.39%	4.062%
33	12.342	3282	3287	3297	rVB2	22620740	35888448	38.19%	2.905%
34	12.413	3297	3309	3317	rBV7	6102430	13844596	14.73%	1.121%

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35	12.493	3318	3334	3340	rBV7	7965568	23483007	24.99%	1.901%
36	12.567	3349	3357	3373	rVB4	26467642	62427754	66.42%	5.054%
37	12.657	3373	3385	3395	rBV6	32206596	67960515	72.31%	5.502%
38	12.738	3396	3410	3419	rBV9	39755800	93985141	100.00%	7.609%
39	12.889	3446	3457	3468	rBV5	13945654	40125119	42.69%	3.248%
40	12.969	3475	3482	3495	rVB4	26637761	53132954	56.53%	4.301%
41	13.046	3495	3506	3516	rBV2	43072969	88138461	93.78%	7.135%
42	13.172	3533	3545	3553	rVB5	11644019	28403602	30.22%	2.299%
43	13.243	3554	3567	3576	rBV5	30355977	65225560	69.40%	5.280%
44	13.291	3577	3582	3590	rVB4	12715031	18690590	19.89%	1.513%
45	13.381	3601	3610	3625	rVB	25186415	46220132	49.18%	3.742%
46	13.545	3656	3661	3668	rVB	14564133	19848917	21.12%	1.607%
47	13.590	3669	3675	3691	rVB4	17348237	37130499	39.51%	3.006%
48	13.670	3691	3700	3710	rBV5	22030851	38390818	40.85%	3.108%
49	13.805	3737	3742	3747	rBV3	6388735	8460421	9.00%	0.685%
50	13.892	3762	3769	3779	rVB	15101734	25167659	26.78%	2.037%
51	13.943	3780	3785	3792	rVB2	3574329	4893534	5.21%	0.396%
52	13.998	3793	3802	3812	rVB4	17802269	30140781	32.07%	2.440%
53	14.056	3812	3820	3823	rBV3	4242299	6604609	7.03%	0.535%
54	14.133	3835	3844	3850	rBV2	5776508	10426622	11.09%	0.844%
55	14.181	3852	3859	3866	rVV5	5184408	9645218	10.26%	0.781%
56	14.252	3876	3881	3889	rVB	8105758	11414975	12.15%	0.924%
57	14.300	3889	3896	3902	rBV3	5368258	7553361	8.04%	0.611%
58	14.339	3902	3908	3915	rVB2	5898323	7818880	8.32%	0.633%
59	14.439	3934	3939	3946	rVB2	3711797	4994597	5.31%	0.404%
60	14.484	3947	3953	3961	rVV4	1770809	3776485	4.02%	0.306%
61	14.529	3963	3967	3975	rVB2	3520932	4497566	4.79%	0.364%
62	14.586	3975	3985	3999	rBV6	10331829	22916710	24.38%	1.855%
63	14.651	4000	4005	4016	rVB2	2831889	4383654	4.66%	0.355%
64	14.744	4027	4034	4044	rVB	4644975	7076260	7.53%	0.573%
65	14.857	4063	4069	4075	rBV3	1346947	1847703	1.97%	0.150%
66	14.956	4093	4100	4113	rVB3	1473676	2992041	3.18%	0.242%
67	15.127	4144	4153	4164	rVB	2689398	4711481	5.01%	0.381%

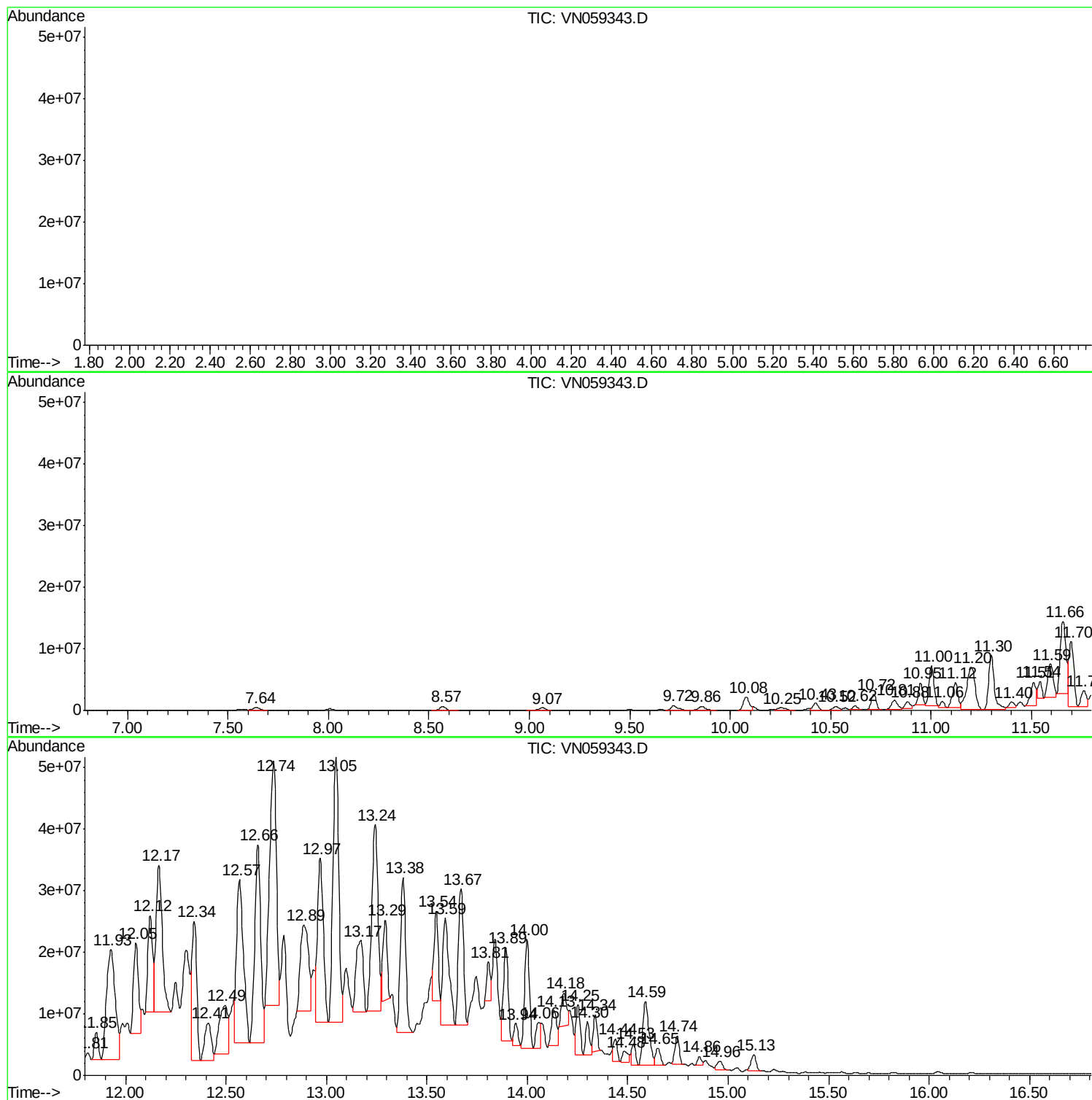
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N112019W.M
Quant Title : SW846 8260

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



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Instrument :
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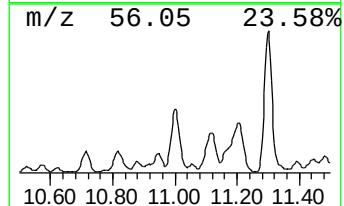
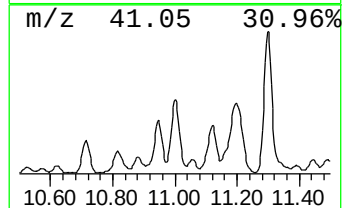
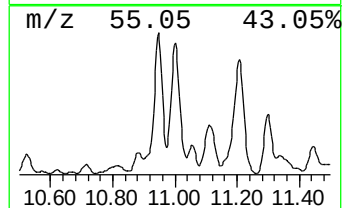
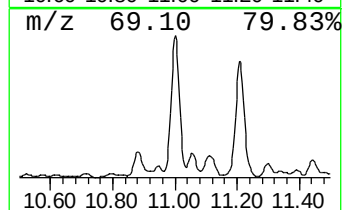
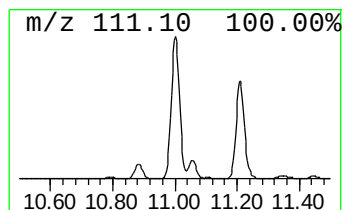
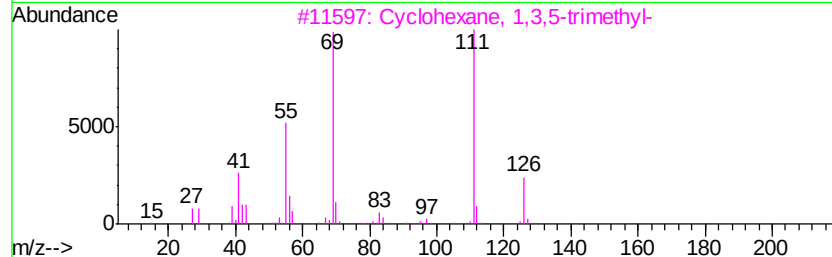
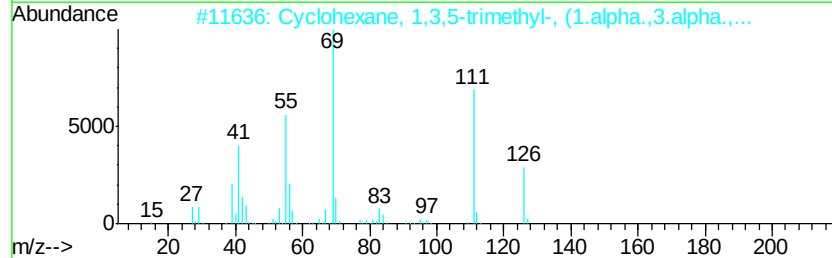
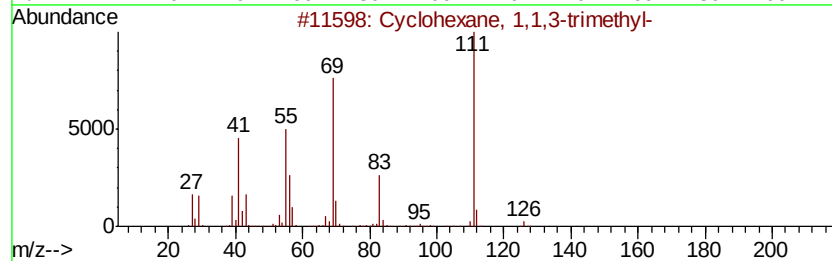
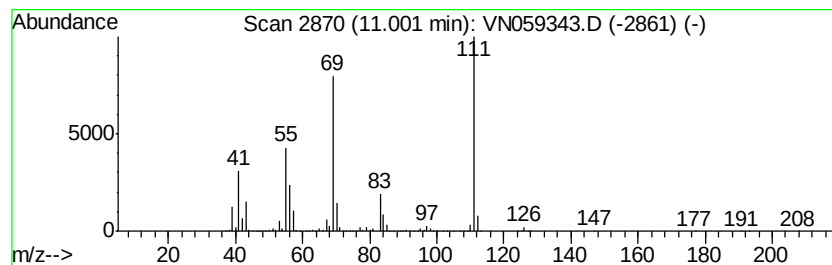
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N112019W.M
Quant Title : SW846 8260

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

Peak Number 1 Cyclohexane, 1,1,3-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.00	380.03 ug/l	11344800	Chlorobenzene-d5	11.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, 1,1,3-trimethyl-	126	C9H18	003073-66-3	95
2		Cyclohexane, 1,3,5-trimethyl-, (...	126	C9H18	001795-26-2	72
3		Cyclohexane, 1,3,5-trimethyl-	126	C9H18	001839-63-0	64
4		2,4,6-Trimethyl-1,5-diazabicyclo...	126	C7H14N2	1000283-21-2	64
5		6-Methyl-hept-2-yn-4-ol	126	C8H14O	060018-69-1	64



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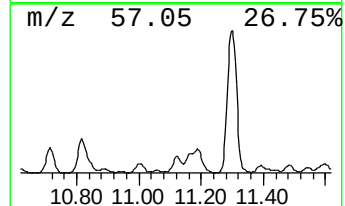
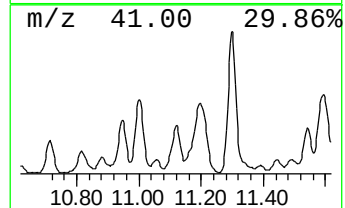
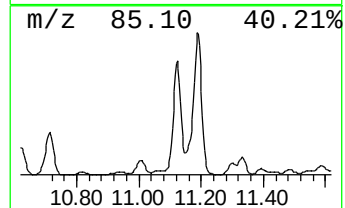
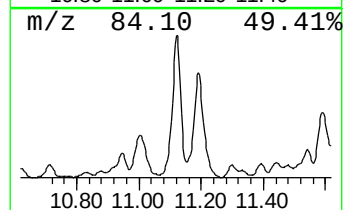
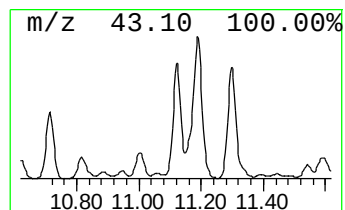
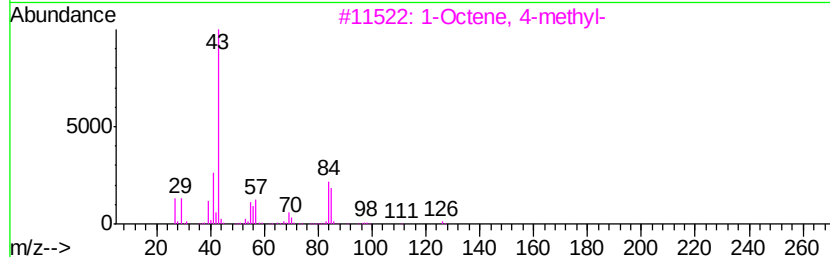
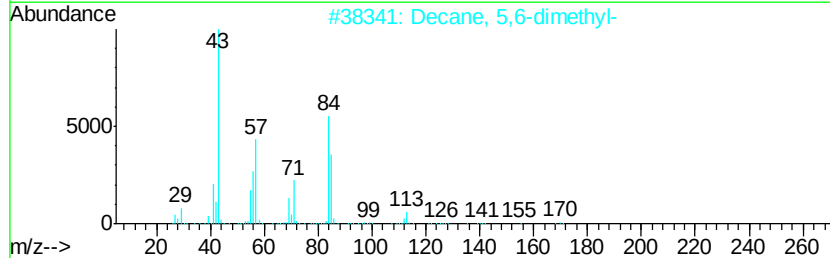
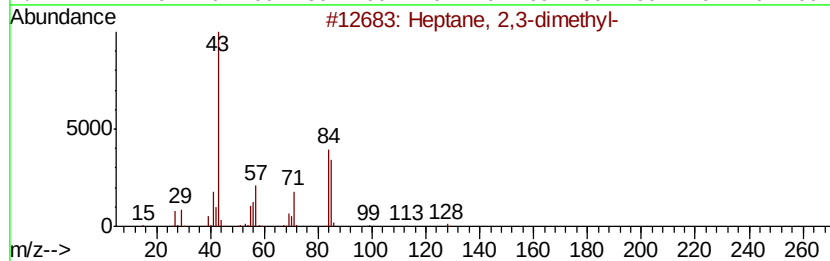
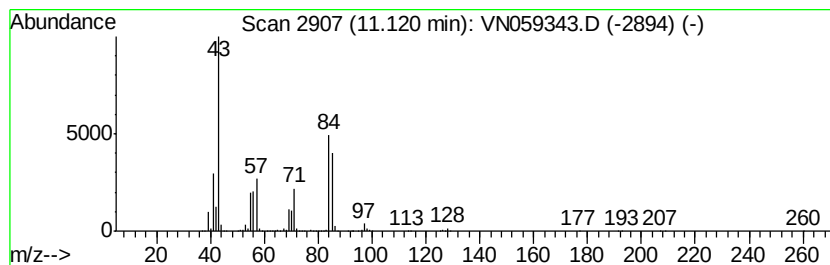
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Heptane, 2,3-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.12	256.91 ug/l	7669440	Chlorobenzene-d5	11.41

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane, 2,3-dimethyl-	128	C9H20	003074-71-3	90	
2	Decane, 5,6-dimethyl-	170	C12H26	001636-43-7	78	
3	1-Octene, 4-methyl-	126	C9H18	013151-12-7	72	
4	Hexane, 2,3,5-trimethyl-	128	C9H20	001069-53-0	58	
5	Hexane, 3-ethyl-2-methyl-	128	C9H20	016789-46-1	58	



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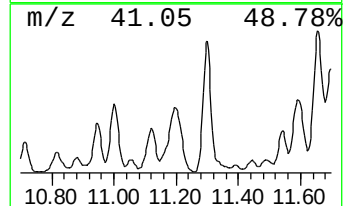
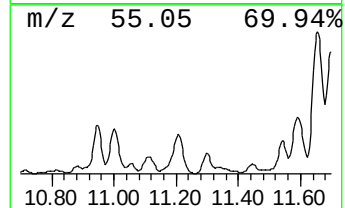
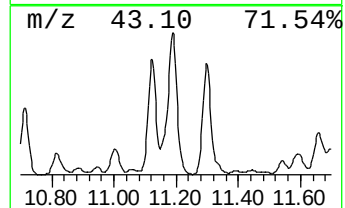
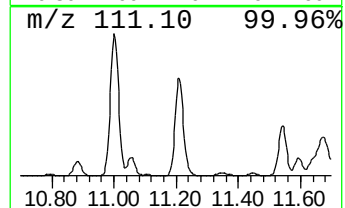
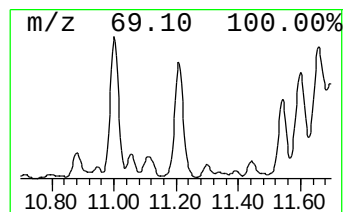
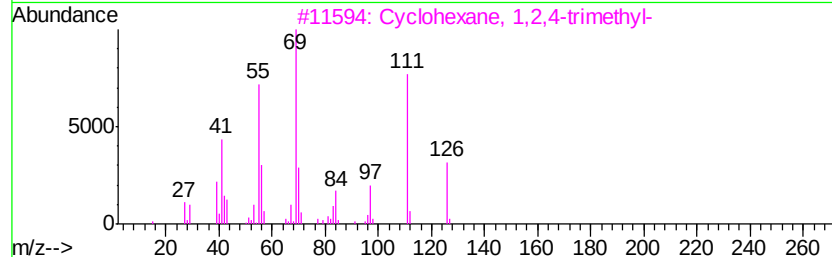
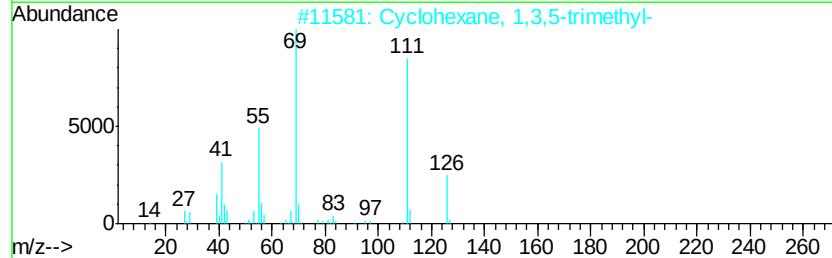
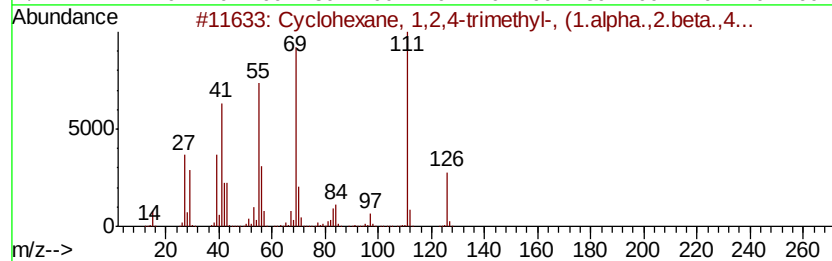
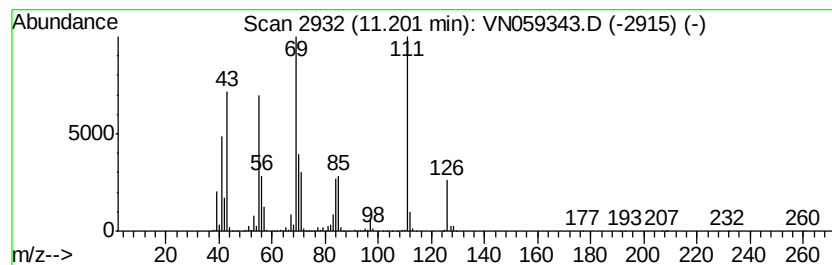
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Peak Number 3 Cyclohexane, 1,2,4-trimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.20	681.59 ug/l	20347000	Chlorobenzene-d5	11.41

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclohexane, 1,2,4-trimethyl-, (...	126	C9H18	007667-60-9	90
2		Cyclohexane, 1,3,5-trimethyl-	126	C9H18	001839-63-0	46
3		Cyclohexane, 1,2,4-trimethyl-	126	C9H18	002234-75-5	46
4		Cyclohexane, 1,3,5-trimethyl-, (...	126	C9H18	001795-27-3	46
5		Cyclohexane, 1,3,5-trimethyl-, (...	126	C9H18	001795-26-2	35



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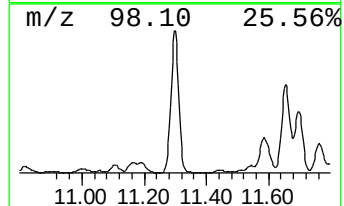
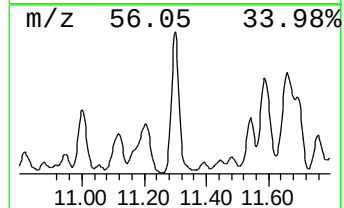
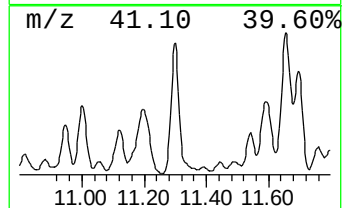
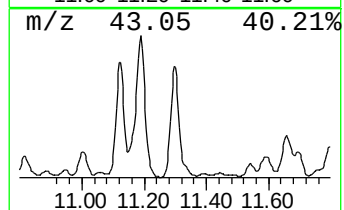
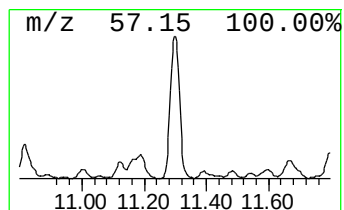
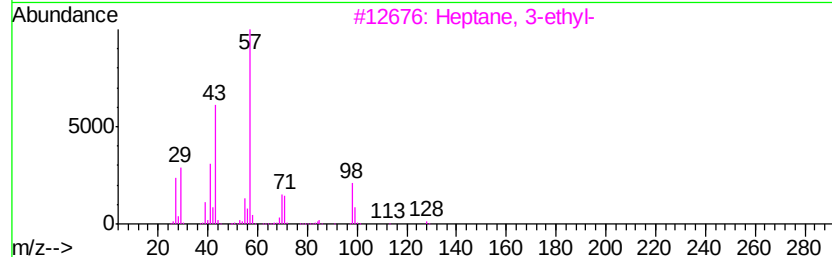
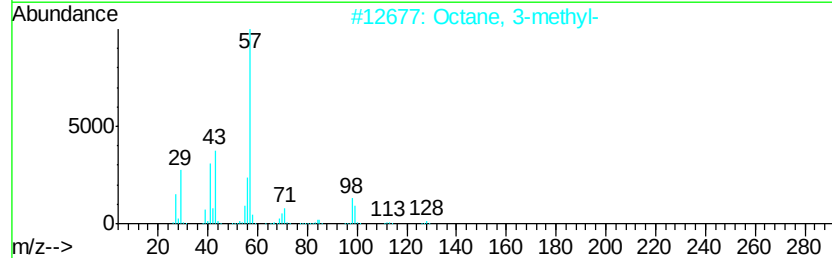
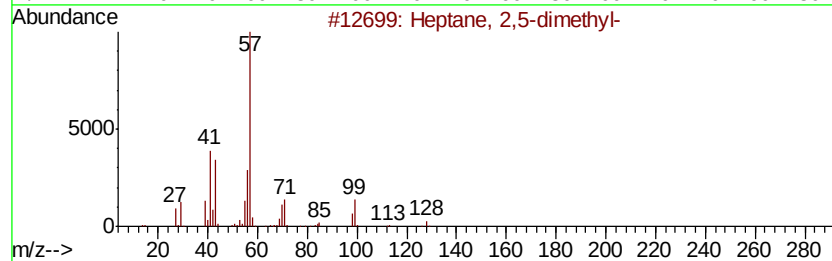
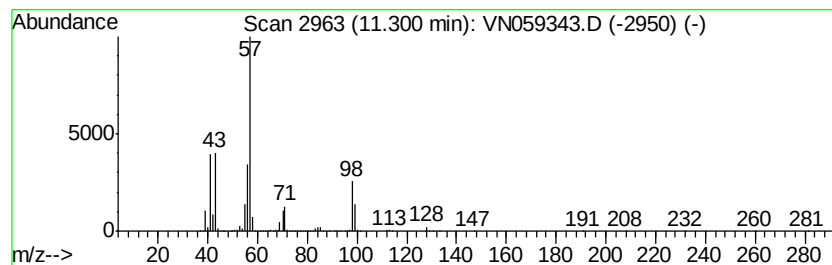
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TIC Integration Parameters: LSCINT.P

Peak Number 4 Heptane, 2,5-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.30	605.45 ug/l	18074000	Chlorobenzene-d5	11.41	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane, 2,5-dimethyl-	128	C9H20	002216-30-0	87
2	Octane, 3-methyl-	128	C9H20	002216-33-3	87
3	Heptane, 3-ethyl-	128	C9H20	015869-80-4	68
4	Heptane, 3,5-dimethyl-	128	C9H20	000926-82-9	62
5	Heptane, 4-propyl-	142	C10H22	003178-29-8	59



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_N\DATA\VN112119\
Data File : VN059343.D
Acq On : 21 Nov 2019 18:02
Operator : JC/SP
Sample : K5957-12
Misc : 5.52a/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-5-(16-18)

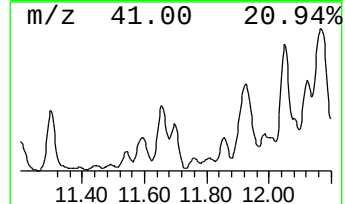
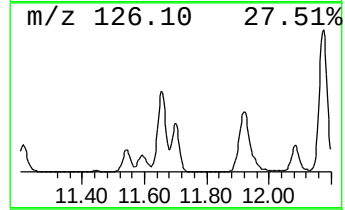
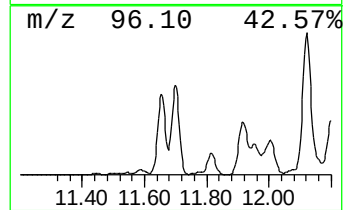
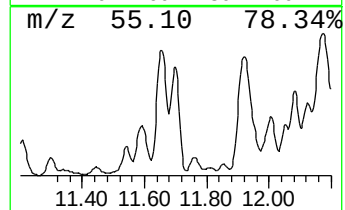
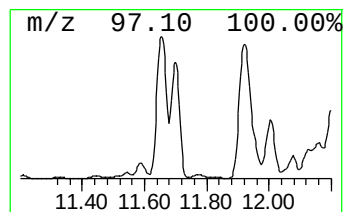
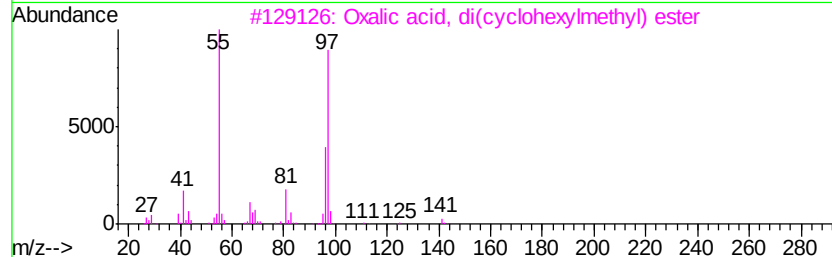
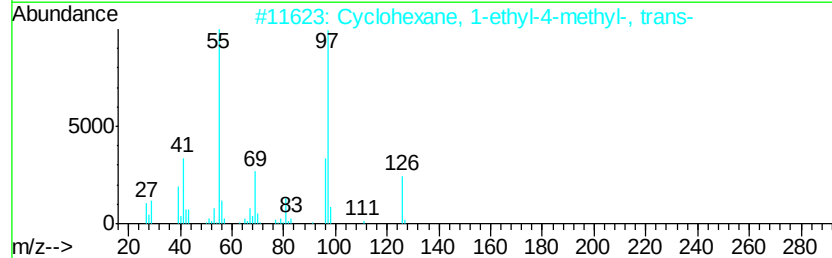
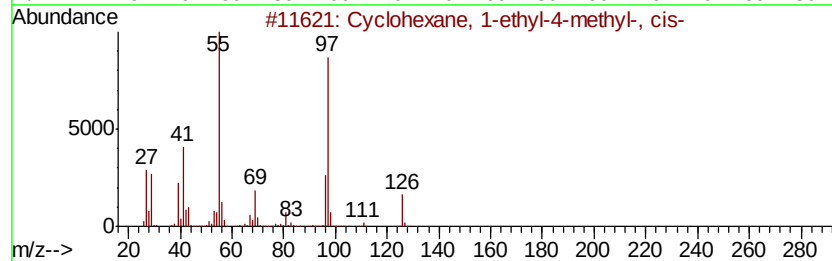
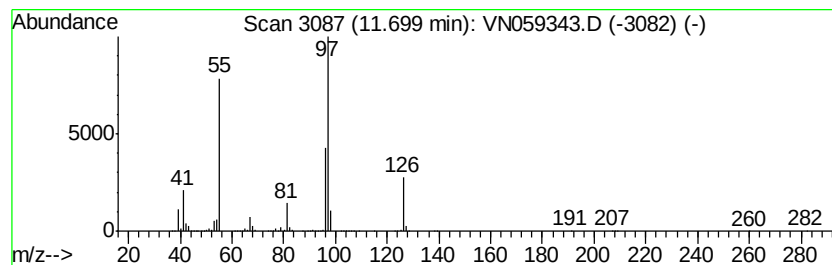
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Quant Title : SW846 8260

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

Peak Number 5 Cyclohexane, 1-ethyl-4-meth... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.70	556.23 ug/l	16604800	Chlorobenzene-d5	11.41

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	004926-78-7	86
2		Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	006236-88-0	83
3		Oxalic acid, di(cyclohexylmethyl)...	282	C16H26O4	1000309-68-5	72
4		1-Ethyl-3-methylcyclohexane (c,t)	126	C9H18	003728-55-0	68
5		cis-1-Ethyl-3-methyl-cyclohexane	126	C9H18	019489-10-2	68



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA N\DATA\VN112119\
Data File : VN059343.D
Acq On : 21 Nov 2019 18:02
Operator : JC/SP
Sample : K5957-12
Misc : 5.52g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 18 Sample Multiplier: 1

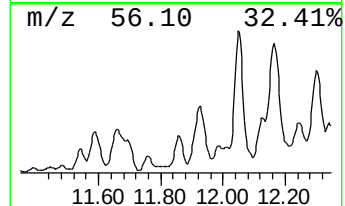
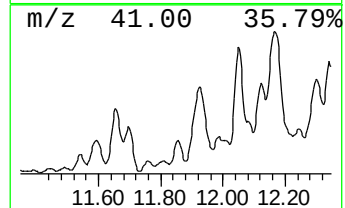
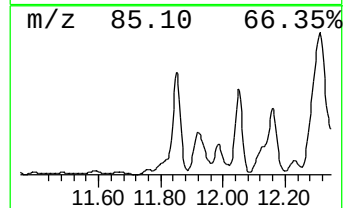
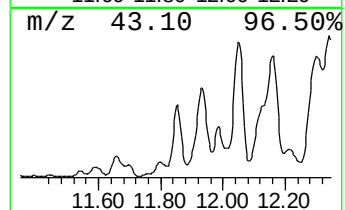
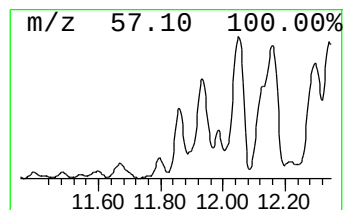
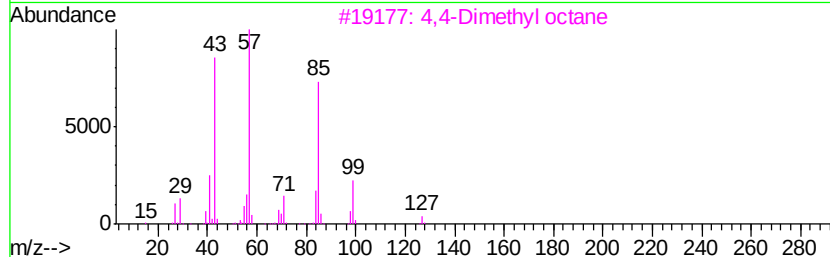
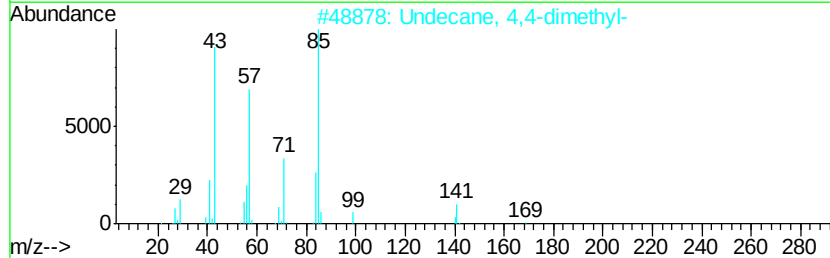
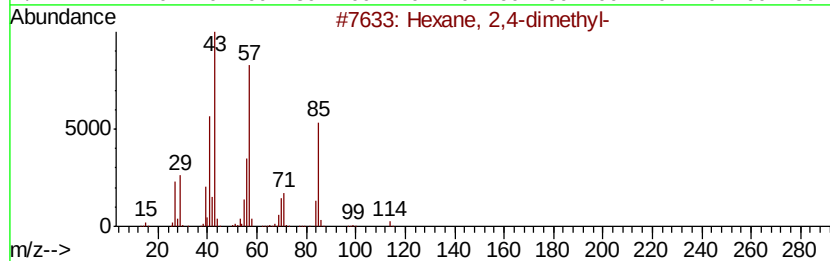
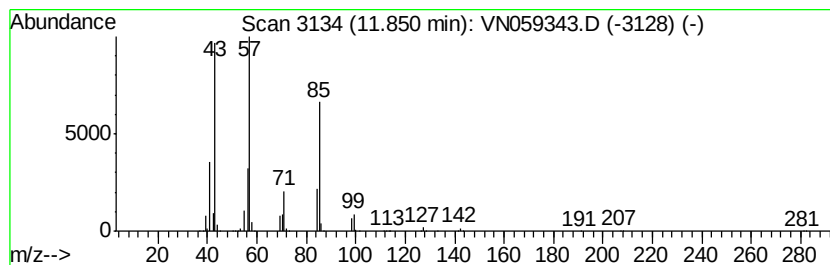
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MSVOA_N
ClientSampleId :
MW-5-(16-18)

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N112019W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.85	218.38 ug/l	6519200	Chlorobenzene-d5	11.41
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Hexane, 2,4-dimethyl-	114 C8H18	000589-43-5	86
2	Undecane, 4,4-dimethyl-	184 C13H28	017312-68-4	64
3	4,4-Dimethyl octane	142 C10H22	015869-95-1	64
4	Sulfurous acid, hexyl heptyl ester	264 C13H28O3S	1000309-12-9	59
5	Octane	114 C8H18	000111-65-9	58



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_N\DATA\VN112119\
Data File : VN059343.D
Acq On : 21 Nov 2019 18:02
Operator : JC/SP
Sample : K5957-12
Misc : 5.52a/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 18 Sample Multiplier: 1

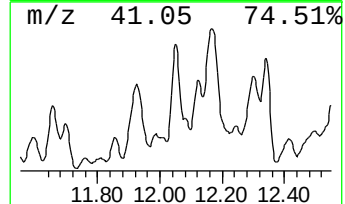
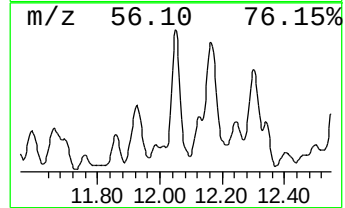
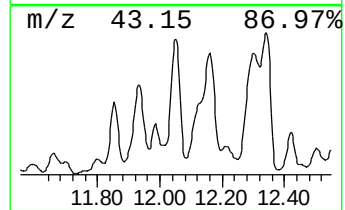
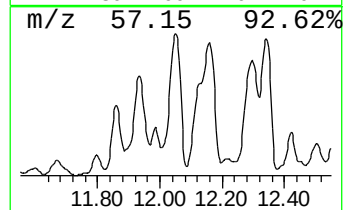
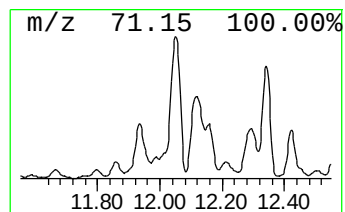
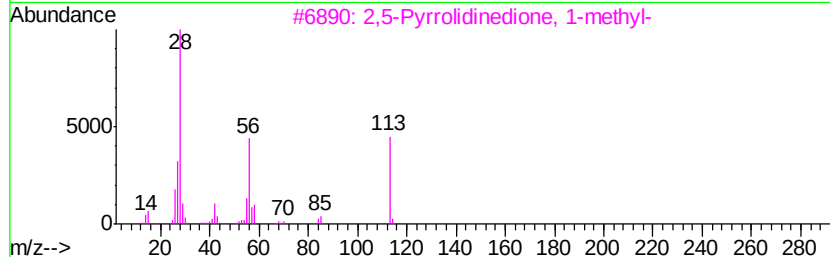
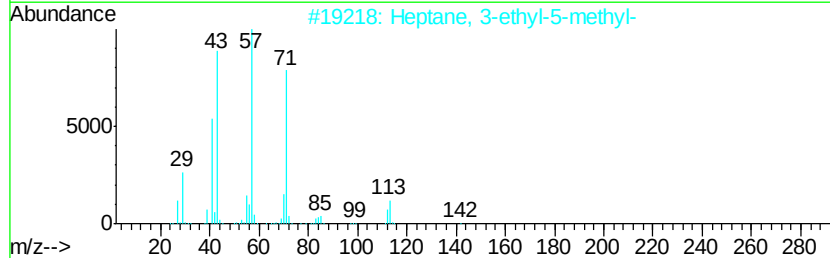
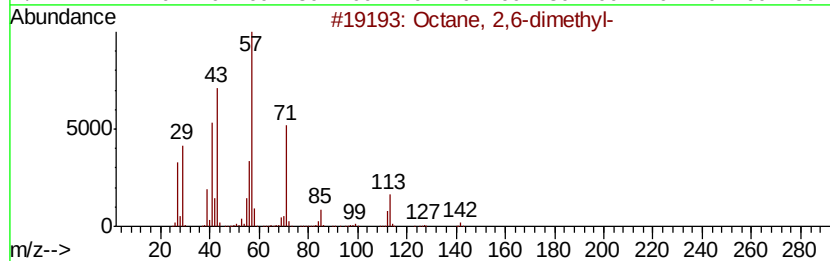
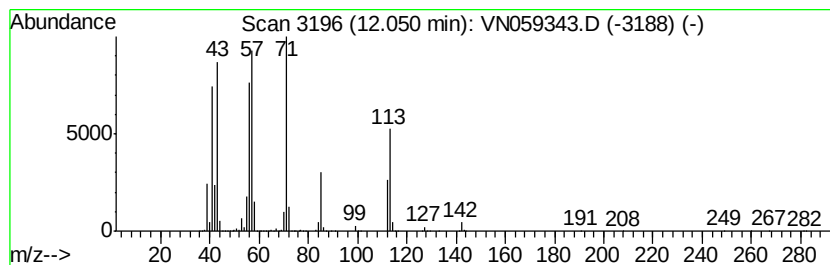
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ClientSampleId :
MW-5-(16-18)

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N112019W.M
Quant Title : SW846 8260

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

Peak Number 7 Octane, 2,6-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.05	842.48 ug/l	25150000	Chlorobenzene-d5	11.41
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Octane, 2,6-dimethyl-	142 C10H22	002051-30-1 64
2		Heptane, 3-ethyl-5-methyl-	142 C10H22	052896-90-9 47
3		2,5-Pyrrolidinedione, 1-methyl-	113 C5H7N02	001121-07-9 43
4		Octane, 3,3-dimethyl-	142 C10H22	004110-44-5 43
5		3-Cyclopentylpropionamide, N-met...	195 C12H21NO	1000340-38-1 38



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_N\DATA\VN112119\
Data File : VN059343.D
Acq On : 21 Nov 2019 18:02
Operator : JC/SP
Sample : K5957-12
Misc : 5.52g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 18 Sample Multiplier: 1

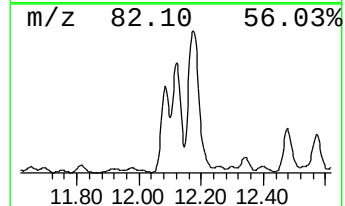
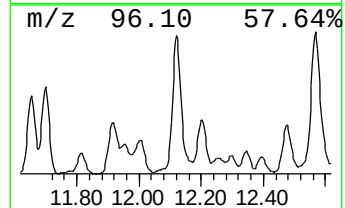
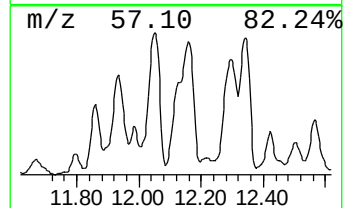
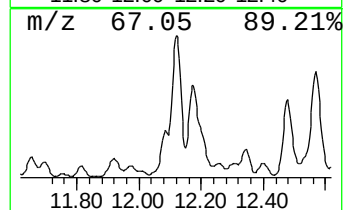
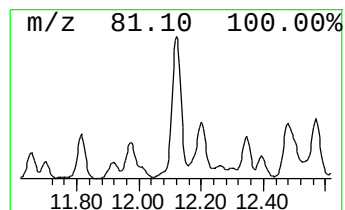
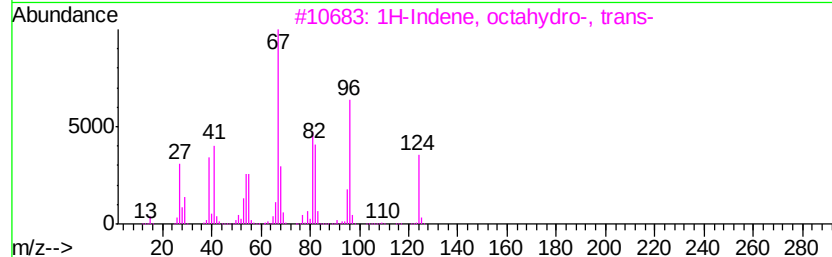
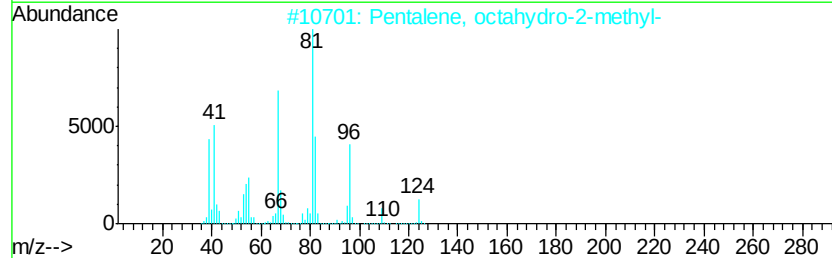
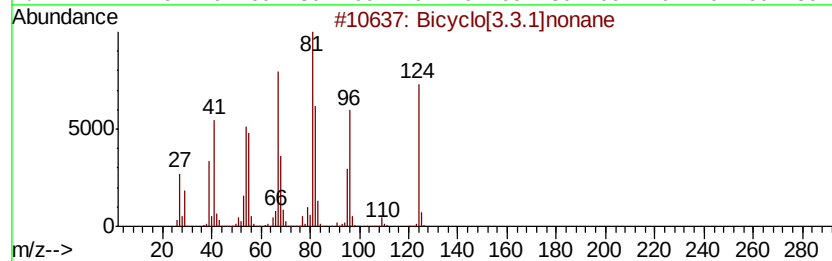
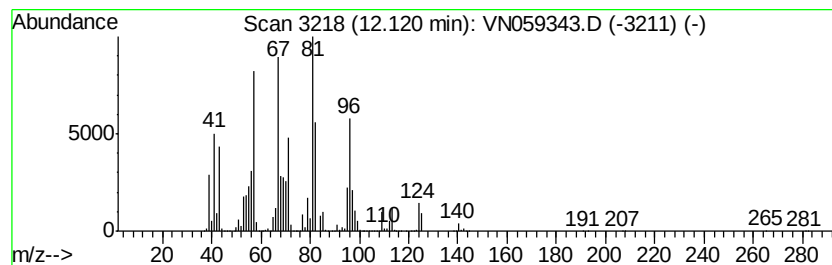
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MW-5-(16-18)

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N112019W.M
Quant Title : SW846 8260

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

Peak Number 8 Bicyclo[3.3.1]nonane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.12	867.39 ug/l	25893400	Chlorobenzene-d5	11.41
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Bicyclo[3.3.1]nonane	124 C9H16	000280-65-9 81
2		Pentalene, octahydro-2-methyl-	124 C9H16	003868-64-2 76
3		1H-Indene, octahydro-, trans-	124 C9H16	003296-50-2 55
4		Cyclohexane, methylene-	96 C7H12	001192-37-6 49
5		Cyclopentane, 1,3-dimethyl-2-(1-...	138 C10H18	061142-31-2 46



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA N\DATA\VN112119\
Data File : VN059343.D
Acq On : 21 Nov 2019 18:02
Operator : JC/SP
Sample : K5957-12
Misc : 5.52g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
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ClientSampleId :
MW-5-(16-18)

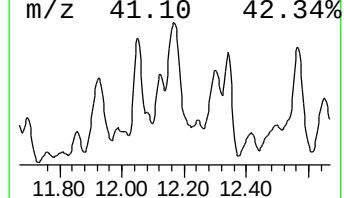
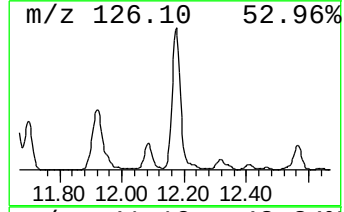
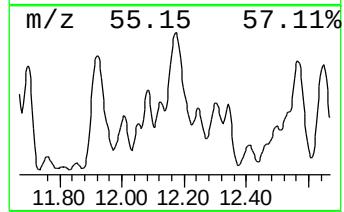
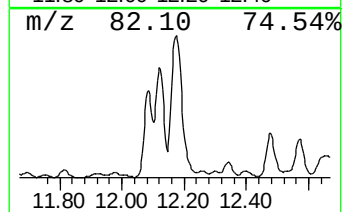
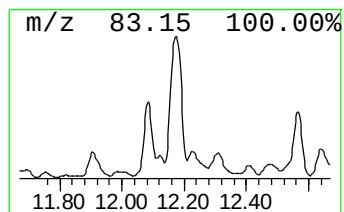
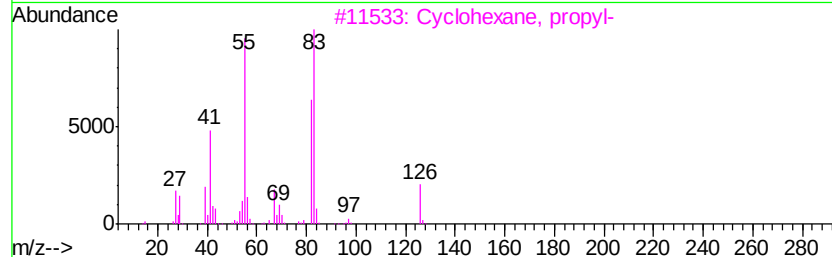
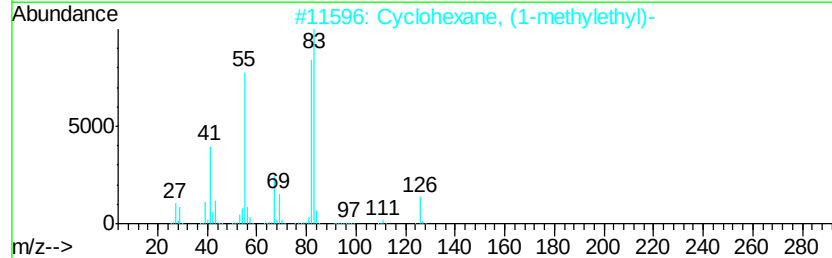
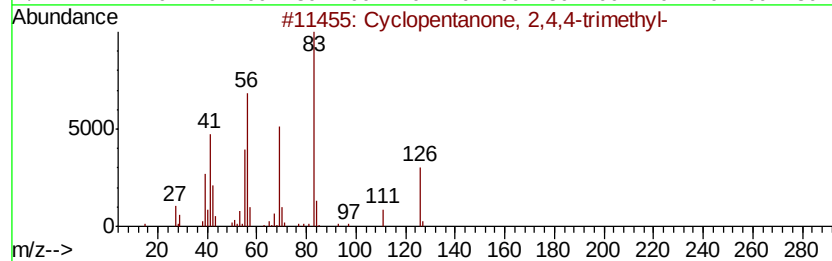
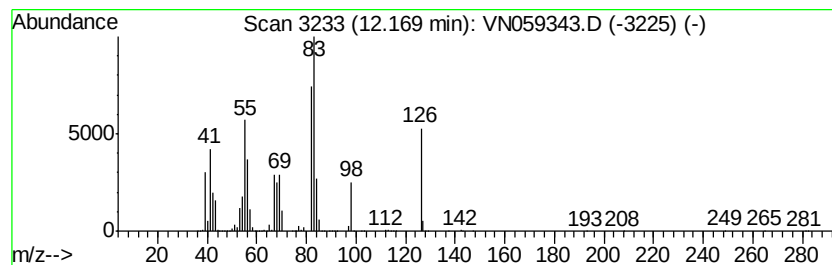
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Quant Title : SW846 8260

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

Peak Number 9 unknown12.17 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.17	1680.86 ug/l	50177600	Chlorobenzene-d5	11.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopentanone, 2,4,4-trimethyl-	126	C8H14O	004694-12-6	47
2		Cyclohexane, (1-methylethyl)-	126	C9H18	000696-29-7	47
3		Cyclohexane, propyl-	126	C9H18	001678-92-8	47
4		2,3-Dimethyl-3-heptene	126	C9H18	1000113-49-3	43
5		Cyclohexane, methyl-	98	C7H14	000108-87-2	43



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN112119\
Data File : VN059343.D
Acq On : 21 Nov 2019 18:02
Operator : JC/SP
Sample : K5957-12
Misc : 5.52a/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 18 Sample Multiplier: 1

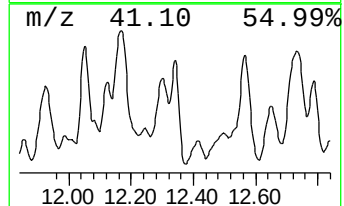
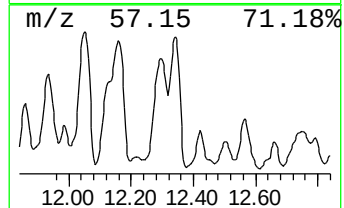
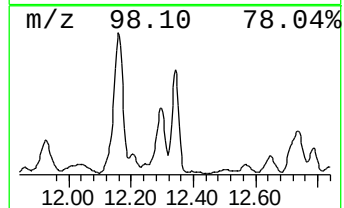
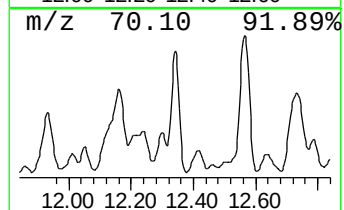
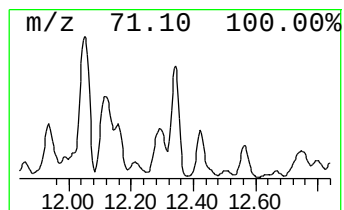
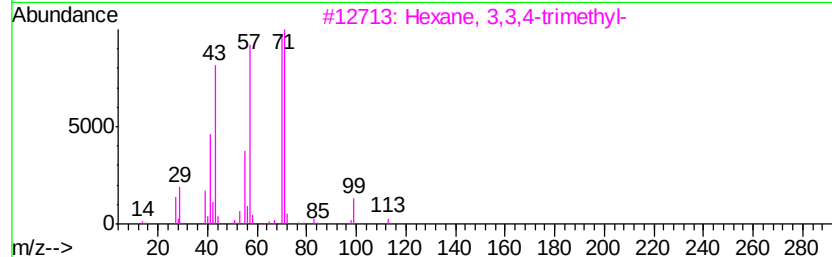
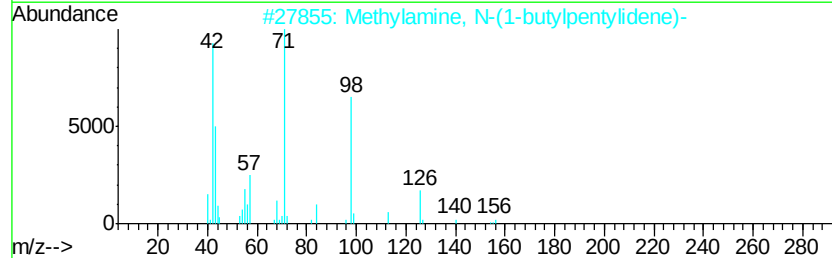
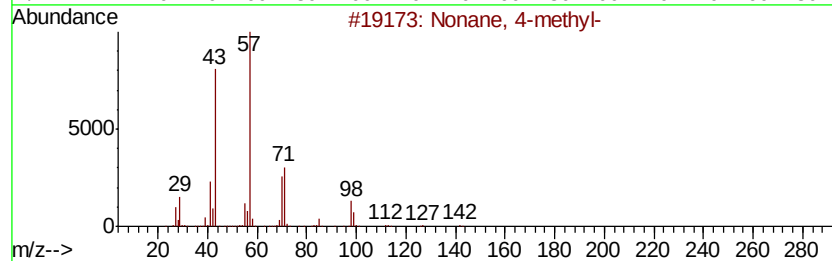
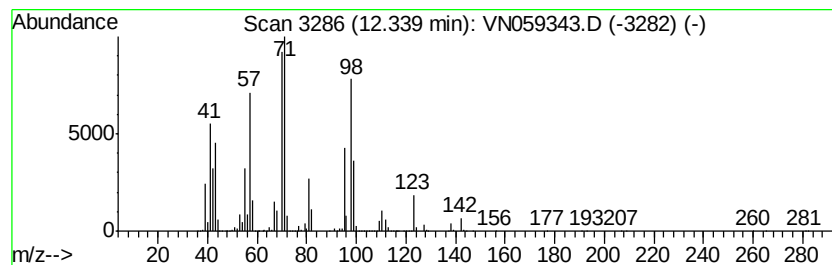
Instrument :
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ClientSampleId :
MW-5-(16-18)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N112019W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.		
12.34	1202.20 ug/l	35888400	Chlorobenzene-d5	11.41		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Nonane, 4-methyl-	142	C10H22	017301-94-9	50
2		Methylamine, N-(1-butylpentylidene...	155	C10H21N	010599-81-2	38
3		Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	32
4		2-Piperidinimine	98	C5H10N2	022780-54-7	27
5		Heptane, 3,3-dimethyl-	128	C9H20	004032-86-4	22



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN112119\
Data File : VN059343.D
Acq On : 21 Nov 2019 18:02
Operator : JC/SP
Sample : K5957-12
Misc : 5.52g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-5-(16-18)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N112019W.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
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Heptane, 2,3-dime...	11.12	256.9	ug/l	7669440	3	11.41	1492610	50.0
Cyclohexane, 1,2,...	11.20	681.6	ug/l	20347000	3	11.41	1492610	50.0
Heptane, 2,5-dime...	11.30	605.5	ug/l	18074000	3	11.41	1492610	50.0
Cyclohexane, 1-et...	11.70	556.2	ug/l	16604800	3	11.41	1492610	50.0
Hexane, 2,4-dimet...	11.85	218.4	ug/l	6519200	3	11.41	1492610	50.0
Octane, 2,6-dimet...	12.05	842.5	ug/l	25150000	3	11.41	1492610	50.0
Bicyclo[3.3.1]nonane	12.12	867.4	ug/l	25893400	3	11.41	1492610	50.0
unknown12.17	12.17	1680.9	ug/l	50177600	3	11.41	1492610	50.0
Nonane, 4-methyl-	12.34	1202.2	ug/l	35888400	3	11.41	1492610	50.0