

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN050219\
 Data File : VN055367.D
 Acq On : 2 May 2019 23:27
 Operator : JC/SP
 Sample : K2658-03 10X
 Misc : 6.49g/5mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 36 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 EP1-SB-E6(14-17)

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\82N042919W.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	7.593	1791	1810	1821	rBV	281670	713366	1.34%	0.172%
2	7.667	1821	1833	1854	rVB	469217	1131920	2.13%	0.272%
3	8.027	1927	1945	1972	rBV2	307254	743649	1.40%	0.179%
4	8.587	2103	2119	2161	rBV	754297	1661884	3.13%	0.400%
5	10.091	2572	2587	2615	rBV2	1540034	3363798	6.33%	0.809%
6	10.432	2685	2693	2710	rVB	404464	752972	1.42%	0.181%
7	10.532	2710	2724	2733	rBV3	240953	532529	1.00%	0.128%
8	10.718	2771	2782	2794	rVB	1347480	2219909	4.18%	0.534%
9	10.821	2800	2814	2826	rBV	715703	1501193	2.83%	0.361%
10	10.886	2826	2834	2841	rVV3	441101	738628	1.39%	0.178%
11	10.950	2845	2854	2862	rVV	1660391	2839212	5.35%	0.683%
12	11.005	2862	2871	2882	rVV2	3066035	5444240	10.25%	1.309%
13	11.124	2895	2908	2916	rBV3	1739985	3237886	6.10%	0.779%
14	11.198	2916	2931	2951	rVB5	2590583	7756652	14.60%	1.865%
15	11.300	2951	2963	2985	rBV	3918729	7190430	13.54%	1.729%
16	11.407	2986	2996	3005	rBV	1032832	1939510	3.65%	0.466%
17	11.506	3016	3027	3031	rBV5	460572	911367	1.72%	0.219%
18	11.542	3032	3038	3044	rVV	1188335	1842611	3.47%	0.443%
19	11.593	3044	3054	3061	rVV5	1993986	4544108	8.55%	1.093%
20	11.654	3065	3073	3081	rVV2	4614747	9255166	17.42%	2.226%
21	11.696	3082	3086	3097	rVB3	3204843	4796428	9.03%	1.153%
22	11.757	3097	3105	3113	rBV3	668112	1249533	2.35%	0.301%
23	11.850	3128	3134	3142	rVB4	914728	1321811	2.49%	0.318%
24	11.921	3142	3156	3169	rBV6	5076423	12624274	23.77%	3.036%
25	12.046	3187	3195	3202	rBV	4912626	6708148	12.63%	1.613%
26	12.120	3210	3218	3223	rBV2	4349853	6976465	13.13%	1.678%
27	12.165	3224	3232	3249	rVV4	8752793	17478643	32.91%	4.203%
28	12.246	3252	3257	3265	rVV4	2204643	3267919	6.15%	0.786%
29	12.297	3267	3273	3279	rVV6	2559952	4551421	8.57%	1.095%
30	12.336	3281	3285	3296	rVB2	5163190	7302574	13.75%	1.756%
31	12.403	3296	3306	3315	rBV7	1959977	3727535	7.02%	0.896%
32	12.487	3315	3332	3338	rBV8	1545606	4813704	9.06%	1.158%
33	12.561	3347	3355	3362	rBV2	6830583	11961196	22.52%	2.877%
34	12.651	3372	3383	3388	rBV6	3748628	7308573	13.76%	1.758%

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35	12.731	3389	3408	3417	rVV6	11930702	37703379	70.98%	9.067%
36	12.779	3418	3423	3433	rVB2	4901270	7391317	13.92%	1.778%
37	12.866	3443	3450	3457	rBV3	2413683	3272173	6.16%	0.787%
38	12.908	3458	3463	3467	rBV2	1097509	1432980	2.70%	0.345%
39	12.960	3473	3479	3493	rVB4	5613634	10069039	18.96%	2.422%
40	13.040	3494	3504	3515	rBV2	32657536	53117484	100.00%	12.774%
41	13.169	3533	3544	3552	rBV3	3841707	7337139	13.81%	1.765%
42	13.236	3553	3565	3574	rVV5	9532470	18695189	35.20%	4.496%
43	13.287	3576	3581	3589	rVB2	3573050	4944890	9.31%	1.189%
44	13.374	3600	3608	3623	rVB	9304970	15231315	28.67%	3.663%
45	13.516	3646	3652	3653	rBV	1598437	1675300	3.15%	0.403%
46	13.541	3654	3660	3667	rVV2	5497303	7748967	14.59%	1.864%
47	13.586	3667	3674	3689	rVB4	6682509	14417499	27.14%	3.467%
48	13.664	3689	3698	3708	rVB4	6302552	11083944	20.87%	2.666%
49	13.802	3734	3741	3745	rBV	3763421	5153240	9.70%	1.239%
50	13.831	3746	3750	3759	rVB	4826689	6458693	12.16%	1.553%
51	13.889	3760	3768	3778	rVB	6940984	10788135	20.31%	2.594%
52	13.943	3780	3785	3790	rBV	613822	705311	1.33%	0.170%
53	13.992	3791	3800	3810	rVB4	6599051	11087572	20.87%	2.666%
54	14.050	3811	3818	3820	rBV3	1044824	1352357	2.55%	0.325%
55	14.127	3835	3842	3849	rVB2	1617560	2218660	4.18%	0.534%
56	14.175	3849	3857	3862	rBV4	1657933	2927090	5.51%	0.704%
57	14.249	3874	3880	3887	rVB	4000080	5589906	10.52%	1.344%
58	14.294	3887	3894	3900	rBV3	1581871	2066538	3.89%	0.497%
59	14.332	3900	3906	3913	rVB2	1572301	1982266	3.73%	0.477%
60	14.432	3932	3937	3944	rVB2	1327269	1827268	3.44%	0.439%
61	14.477	3944	3951	3959	rVV4	747981	1571623	2.96%	0.378%
62	14.522	3960	3965	3973	rVB2	1362809	1940320	3.65%	0.467%
63	14.580	3973	3983	3997	rBV2	4655352	8754024	16.48%	2.105%
64	14.648	3997	4004	4014	rBV	698370	1153768	2.17%	0.277%
65	14.741	4025	4033	4041	rVB	1066379	1551770	2.92%	0.373%
66	14.850	4061	4067	4072	rBV3	493035	672062	1.27%	0.162%
67	14.956	4091	4100	4118	rVB3	660834	1485991	2.80%	0.357%

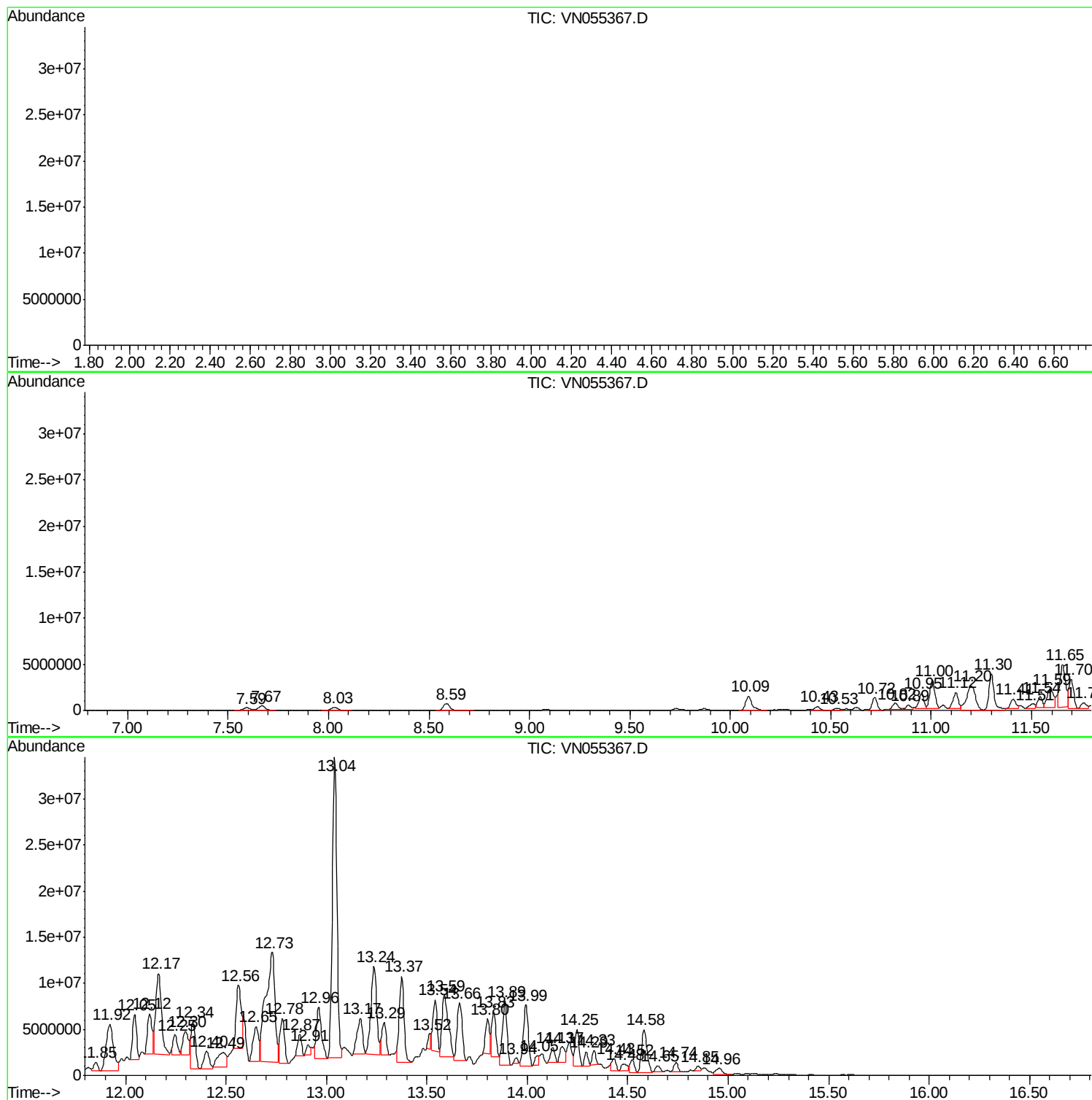
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N042919W.M
Quant Title : SW846 8260

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



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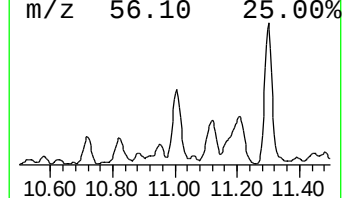
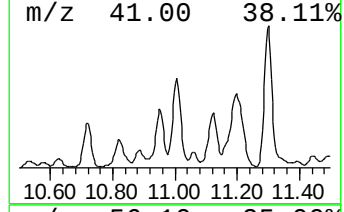
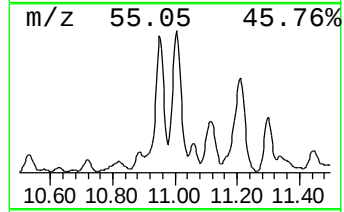
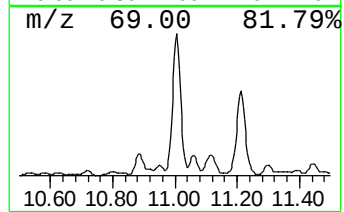
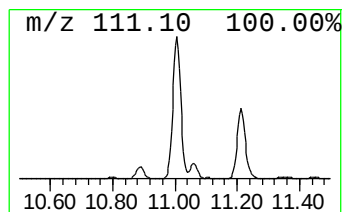
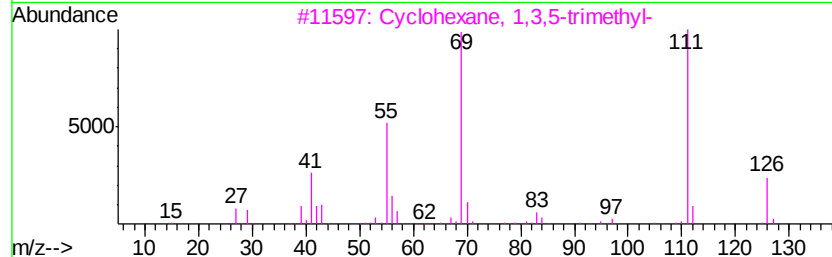
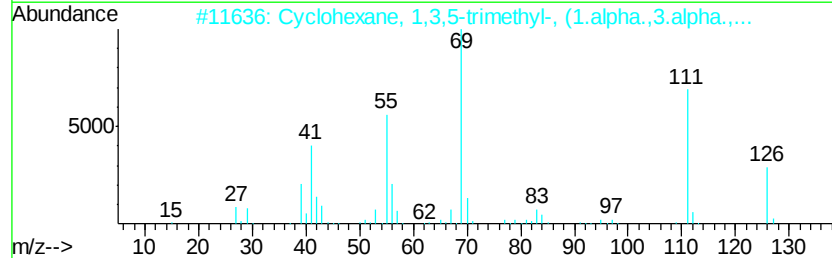
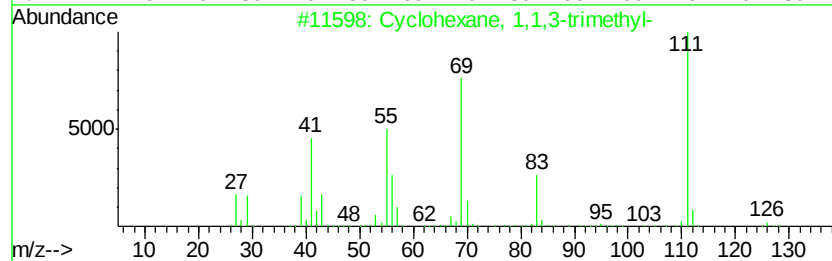
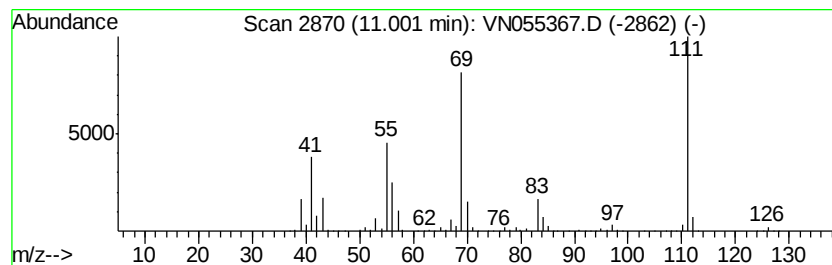
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N042919W.M
Quant Title : SW846 8260

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	140.35 ug/l	5444240	Chlorobenzene-d5	11.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, 1,1,3-trimethyl-	126	C9H18	003073-66-3	91
2		Cyclohexane, 1,3,5-trimethyl-, (...)	126	C9H18	001795-26-2	78
3		Cyclohexane, 1,3,5-trimethyl-	126	C9H18	001839-63-0	72
4		1-Hexene, 3,3-dimethyl-	112	C8H16	003404-77-1	46
5		3-Hexene, 2,5-dimethyl-	112	C8H16	015910-22-2	46



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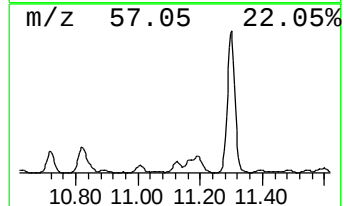
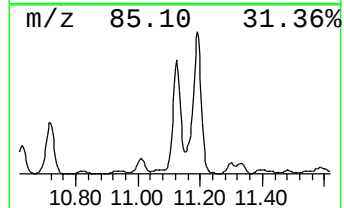
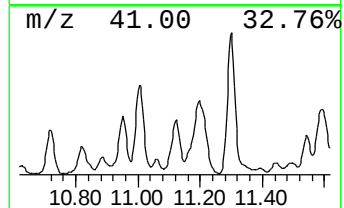
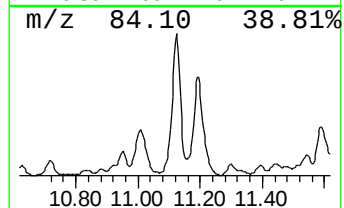
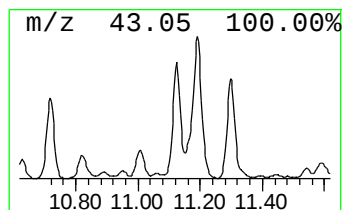
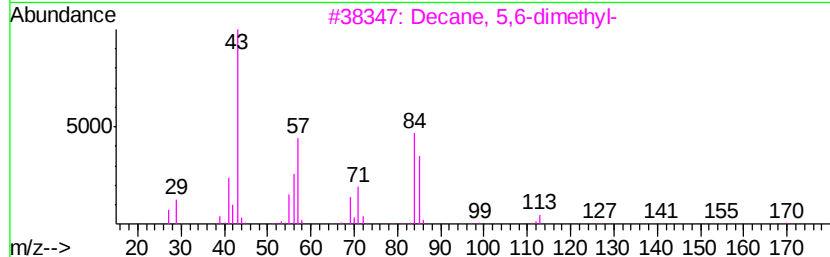
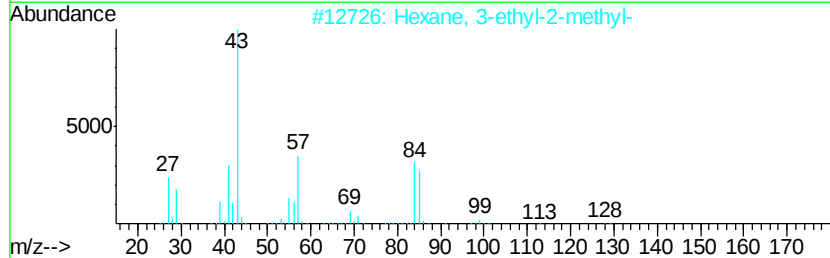
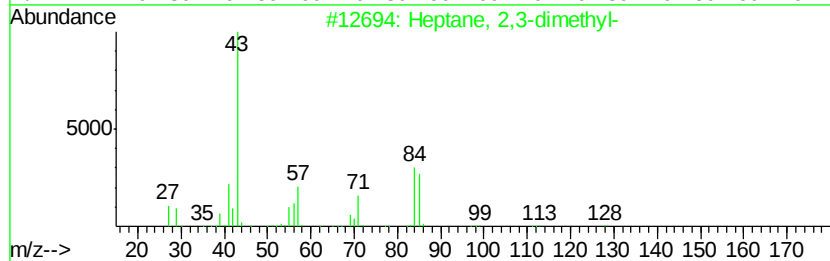
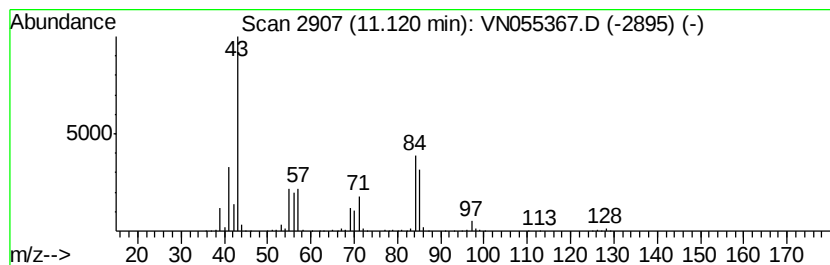
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TIC Integration Parameters: LSCINT.P

Peak Number 2 Heptane, 2,3-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.		
11.12	83.47 ug/l	3237890	Chlorobenzene-d5	11.41		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptane, 2,3-dimethyl-	128	C9H20	003074-71-3	91
2		Hexane, 3-ethyl-2-methyl-	128	C9H20	016789-46-1	90
3		Decane, 5,6-dimethyl-	170	C12H26	001636-43-7	83
4		Nonane, 4,5-dimethyl-	156	C11H24	017302-23-7	56
5		Hexane, 2,3,5-trimethyl-	128	C9H20	001069-53-0	52



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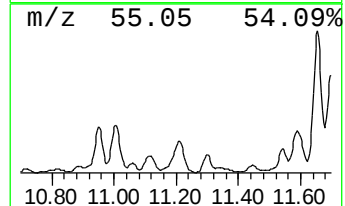
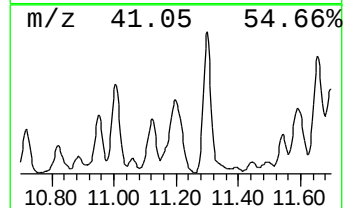
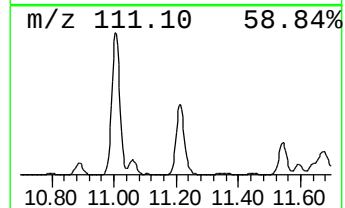
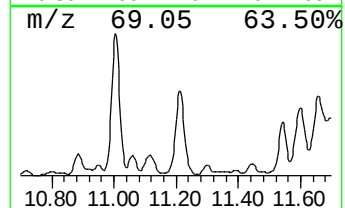
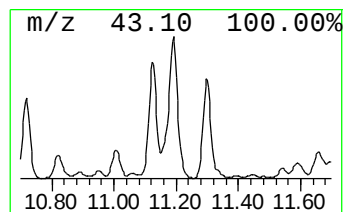
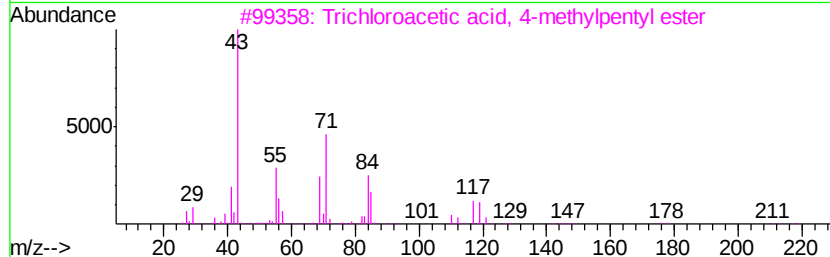
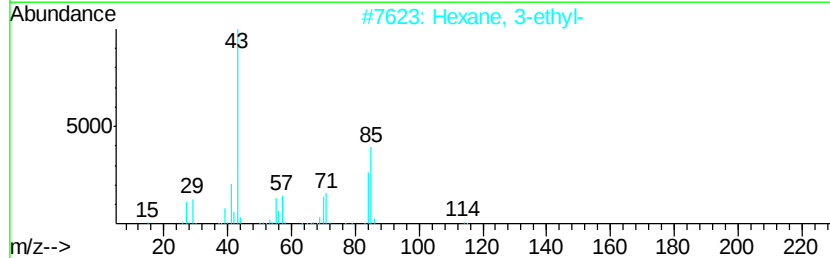
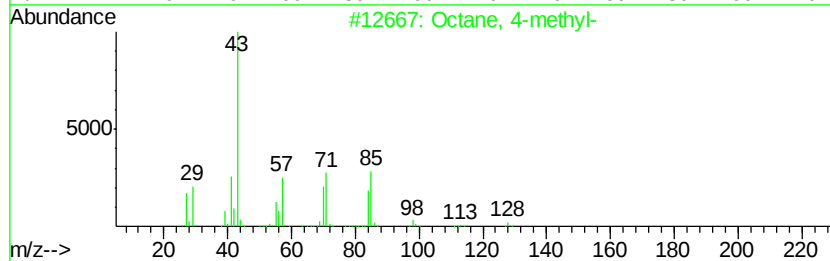
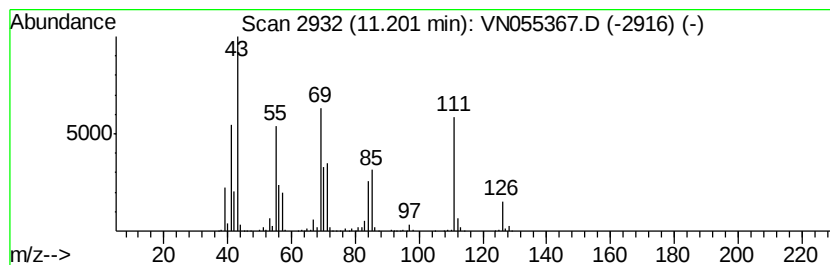
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Peak Number 3 Octane, 4-methyl- Concentration Rank 3

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11.20	199.96 ug/l	7756650	Chlorobenzene-d5	11.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octane, 4-methyl-	128	C9H20	002216-34-4	72
2		Hexane, 3-ethyl-	114	C8H18	000619-99-8	59
3		Trichloroacetic acid, 4-methylpe...	246	C8H13Cl3O2	1000282-35-2	47
4		Octane	114	C8H18	000111-65-9	47
5		1-Pentanol, 2-methyl-	102	C6H14O	000105-30-6	47



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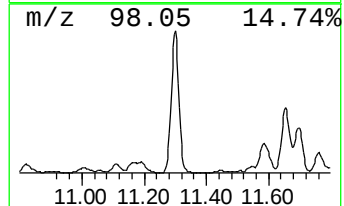
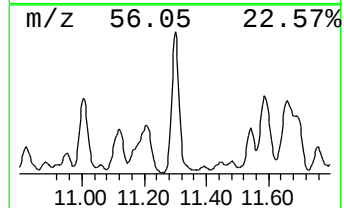
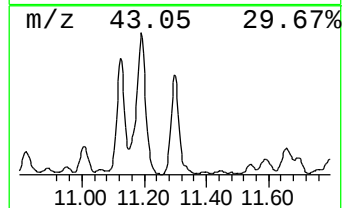
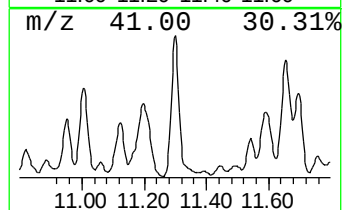
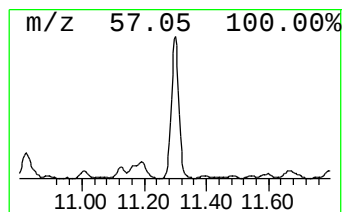
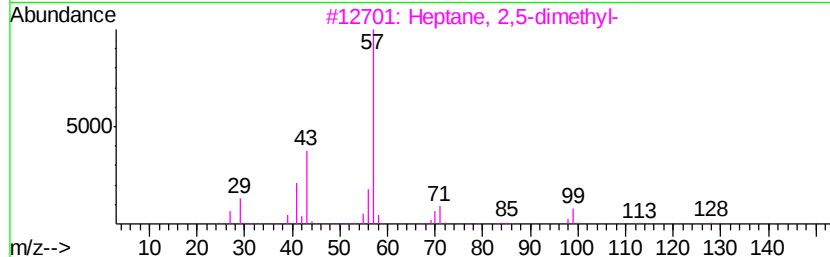
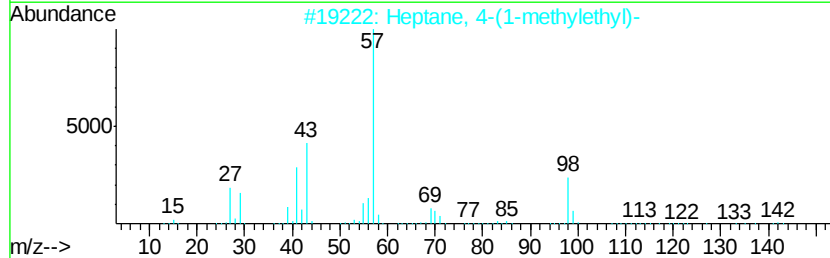
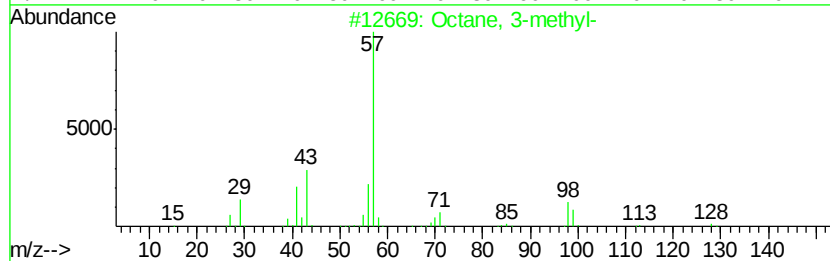
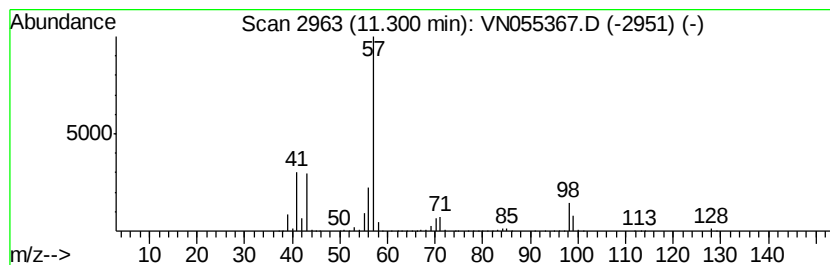
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 TIC Integration Parameters: LSCINT.P

 Peak Number 4 Octane, 3-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.30	185.37 ug/l	7190430	Chlorobenzene-d5	11.41	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 3-methyl-	128	C9H20	002216-33-3	91
2	Heptane, 4-(1-methylethyl)-	142	C10H22	052896-87-4	64
3	Heptane, 2,5-dimethyl-	128	C9H20	002216-30-0	64
4	Oxalic acid, isobutyl heptyl ester	244	C13H24O4	1000309-37-2	59
5	Undecane, 6-methyl-	170	C12H26	017302-33-9	53



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_N\DATA\VN050219\
Data File : VN055367.D
Acq On : 2 May 2019 23:27
Operator : JC/SP
Sample : K2658-03 10X
Misc : 6.49g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 36 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
EP1-SB-E6(14-17)

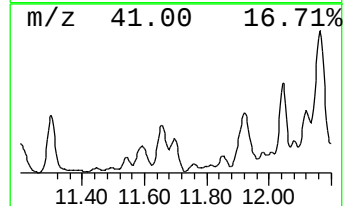
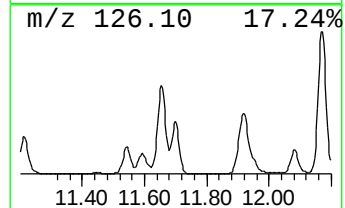
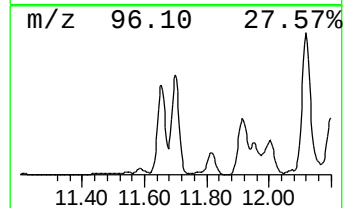
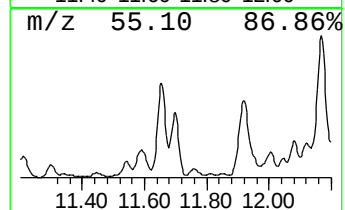
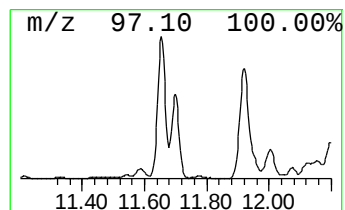
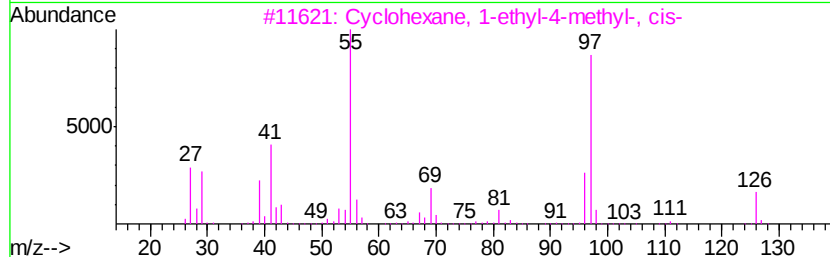
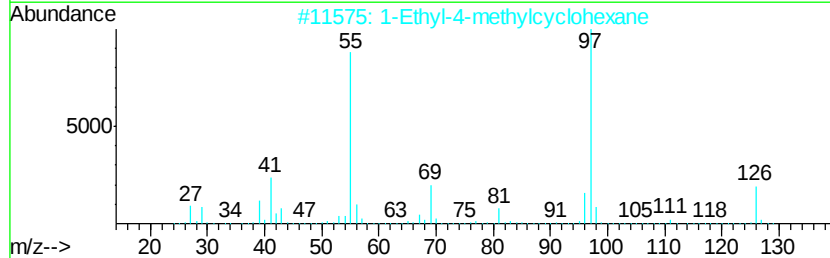
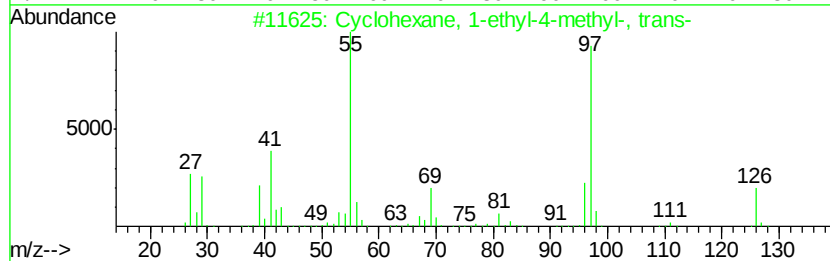
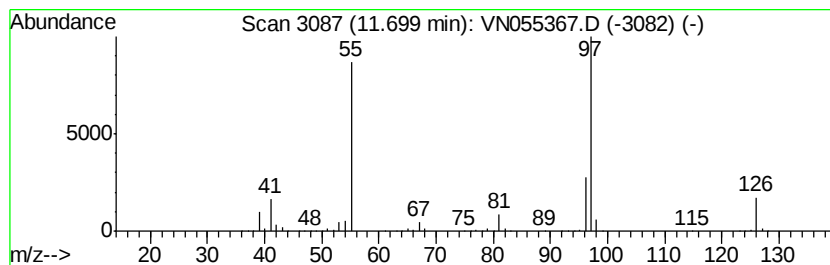
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Quant Title : SW846 8260

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

Peak Number 5 Cyclohexane, 1-ethyl-4-meth... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.70	123.65 ug/l	4796430	Chlorobenzene-d5	11.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	006236-88-0	90
2		1-Ethyl-4-methylcyclohexane	126	C9H18	003728-56-1	87
3		Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	004926-78-7	83
4		Cyclohexane, 1-ethyl-1-methyl-	126	C9H18	004926-90-3	72
5		Cyclopentane, 1-hydroxymethyl-1,...	128	C8H16O	1000156-73-8	72



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_N\DATA\VN050219\
Data File : VN055367.D
Acq On : 2 May 2019 23:27
Operator : JC/SP
Sample : K2658-03 10X
Misc : 6.49g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 36 Sample Multiplier: 1

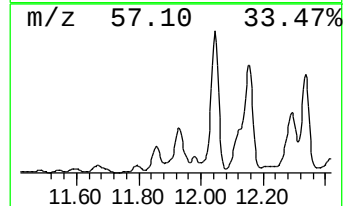
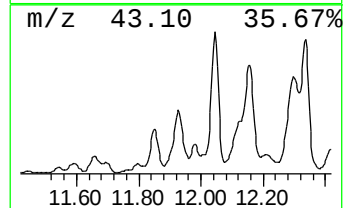
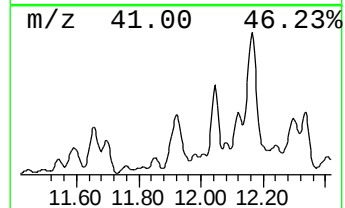
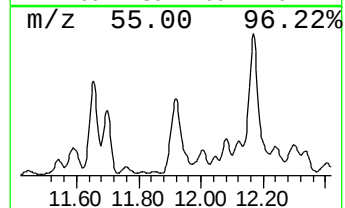
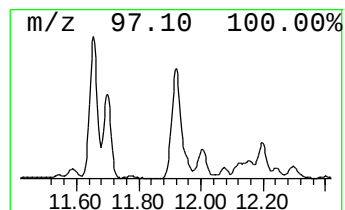
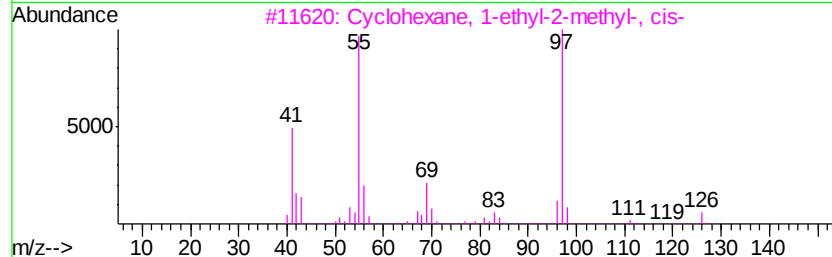
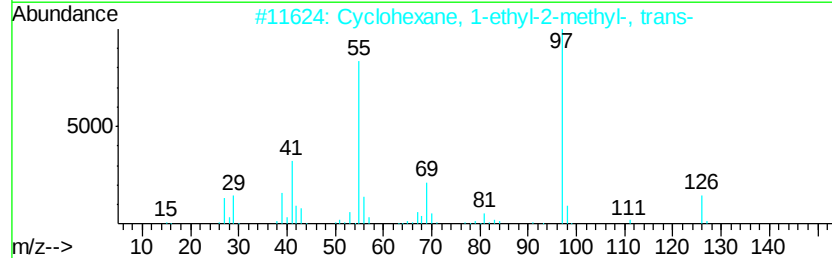
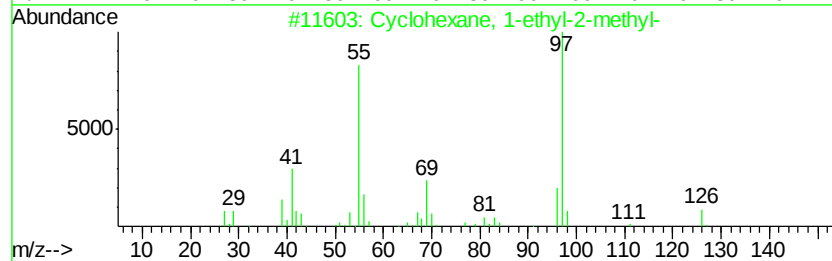
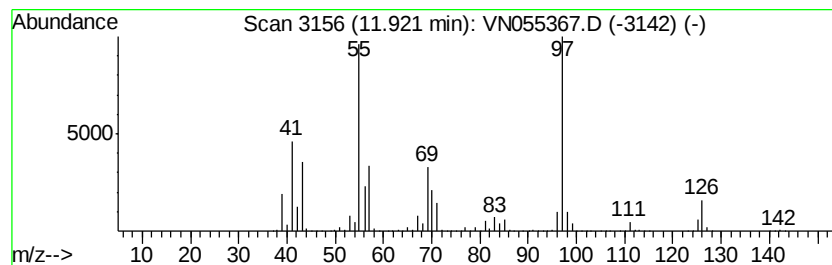
Instrument :
MSVOA_N
ClientSampleId :
EP1-SB-E6(14-17)

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N042919W.M
Quant Title : SW846 8260

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

Peak Number 6 Cyclohexane, 1-ethyl-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.		
11.92	325.45 ug/l	12624300	Chlorobenzene-d5	11.41		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cvclohexane, 1-ethyl-2-methyl-	126	C9H18	003728-54-9	81
2		Cvclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-78-8	68
3		Cvclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-77-7	64
4		Sulfurous acid, cvclohexvlmethyl...	402	C23H46O3S	1000309-22-4	64
5		Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	006236-88-0	64



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_N\DATA\VN050219\
Data File : VN055367.D
Acq On : 2 May 2019 23:27
Operator : JC/SP
Sample : K2658-03 10X
Misc : 6.49g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 36 Sample Multiplier: 1

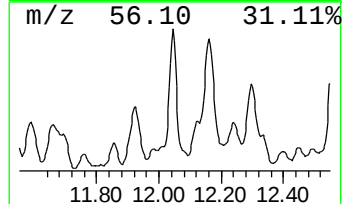
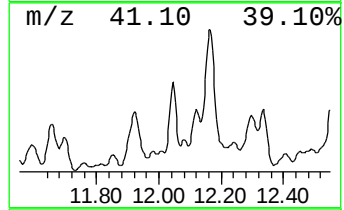
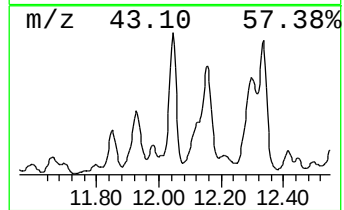
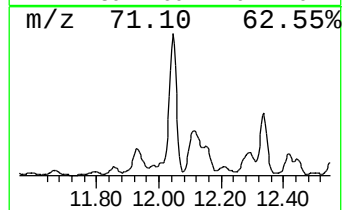
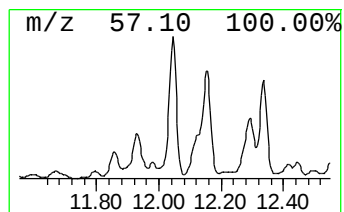
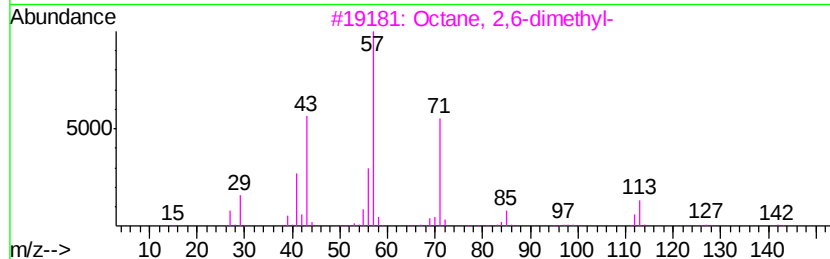
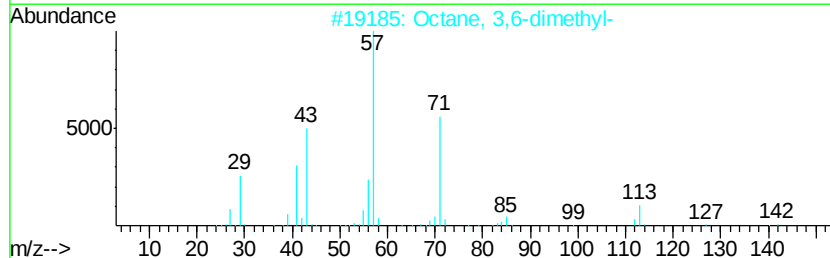
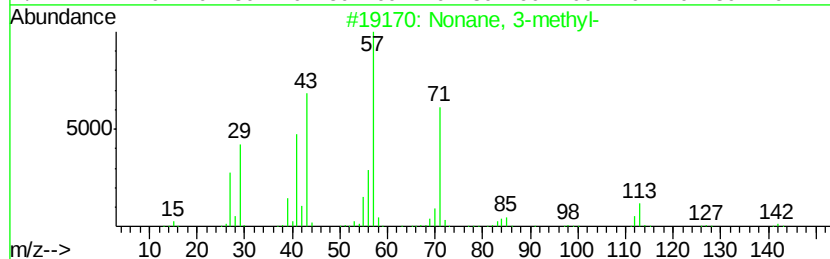
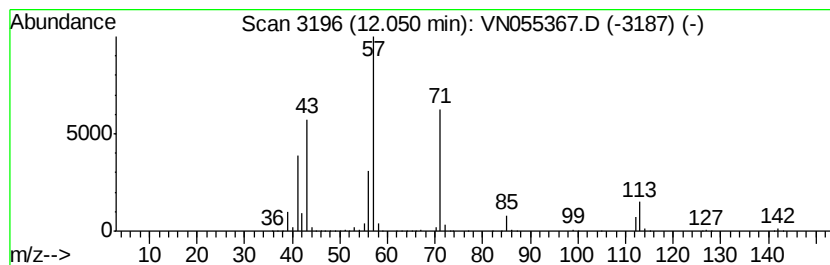
Instrument :
MSVOA_N
ClientSampleId :
EP1-SB-E6(14-17)

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N042919W.M
Quant Title : SW846 8260

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

Peak Number 7 Nonane, 3-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.		
12.05	172.93 ug/l	6708150	Chlorobenzene-d5	11.41		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonane, 3-methyl-		142	C10H22	005911-04-6	91
2	Octane, 3,6-dimethyl-		142	C10H22	015869-94-0	91
3	Octane, 2,6-dimethyl-		142	C10H22	002051-30-1	91
4	Sulfurous acid, 2-ethylhexyl iso...		278	C14H30O3S	1000309-19-0	64
5	Decane, 2,6,7-trimethyl-		184	C13H28	062108-25-2	64



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA N\DATA\VN050219\
Data File : VN055367.D
Acq On : 2 May 2019 23:27
Operator : JC/SP
Sample : K2658-03 10X
Misc : 6.49µ/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 36 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
EP1-SB-E6(14-17)

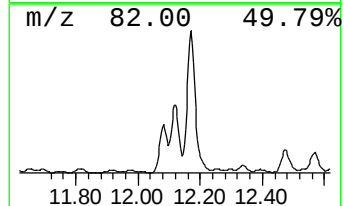
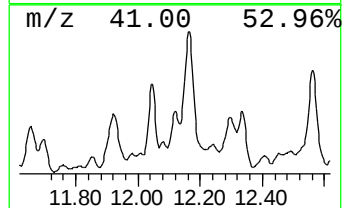
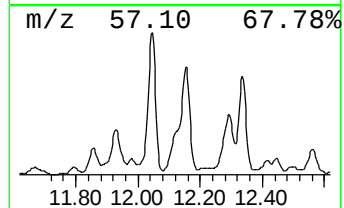
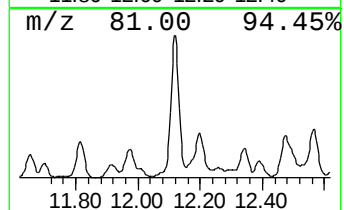
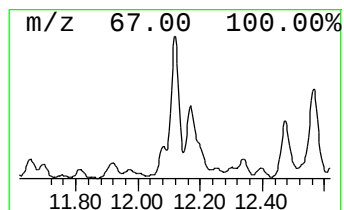
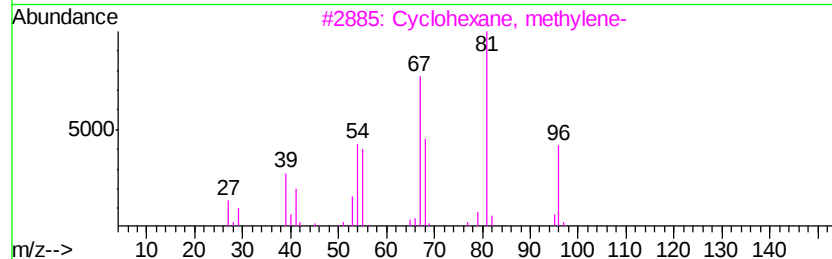
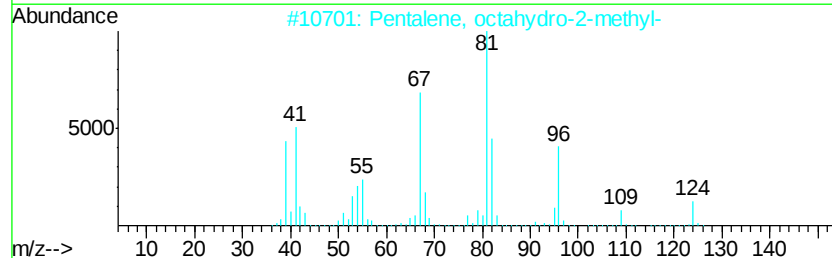
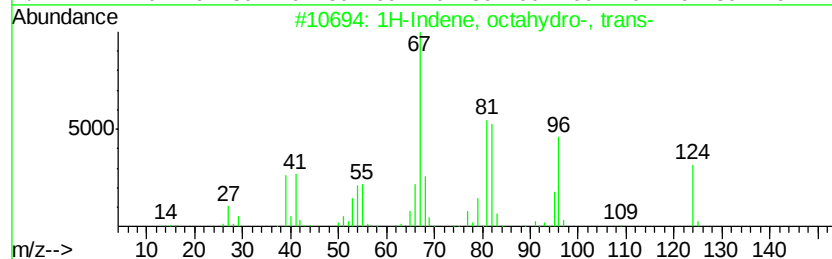
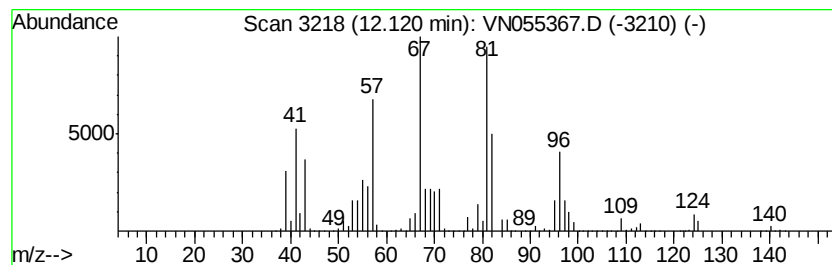
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Quant Title : SW846 8260

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

Peak Number 8 1H-Indene, octahydro-, trans- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.12	179.85 ug/l	6976470	Chlorobenzene-d5	11.41

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1H-Indene, octahydro-, trans-	124	C9H16	003296-50-2	53
2		Pentalene, octahydro-2-methyl-	124	C9H16	003868-64-2	53
3		Cyclohexane, methylene-	96	C7H12	001192-37-6	52
4		Cyclohexene, 1-methyl-	96	C7H12	000591-49-1	49
5		Propylidencyclohexane	124	C9H16	002129-93-3	43



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_N\DATA\VN050219\
Data File : VN055367.D
Acq On : 2 May 2019 23:27
Operator : JC/SP
Sample : K2658-03 10X
Misc : 6.49g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 36 Sample Multiplier: 1

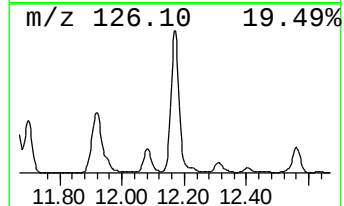
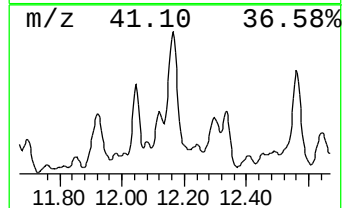
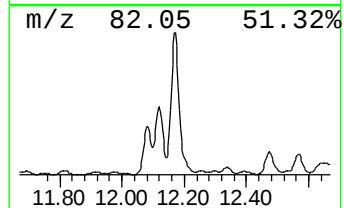
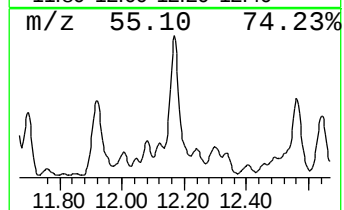
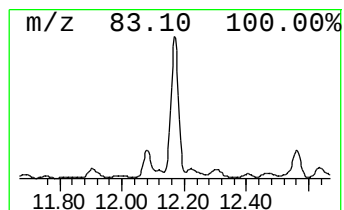
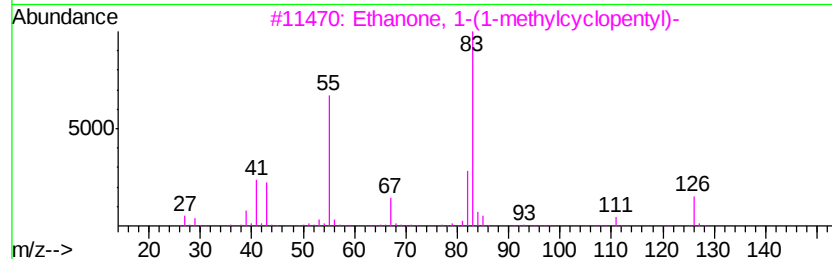
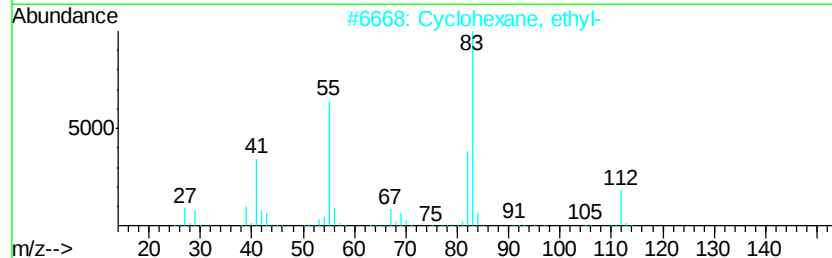
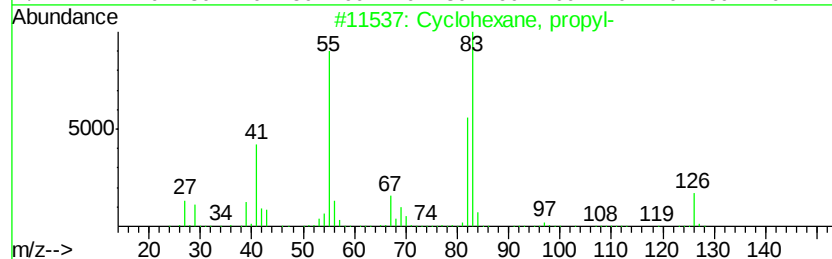
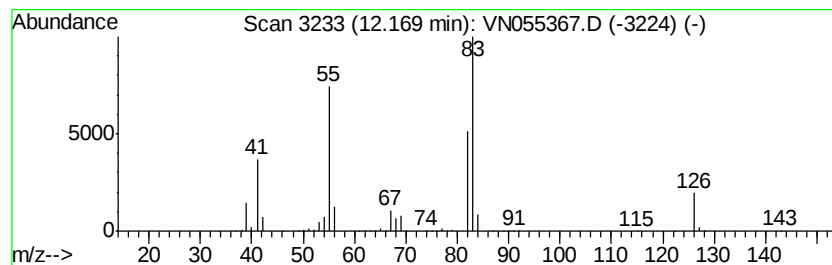
Instrument :
MSVOA_N
ClientSampleID :
EP1-SB-E6(14-17)

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N042919W.M
Quant Title : SW846 8260

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

Peak Number 9 Cyclohexane, propyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.		
12.17	450.59 ug/l	17478600	Chlorobenzene-d5	11.41		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cvclohexane, propyl-	126	C9H18	001678-92-8	90
2		Cvclohexane, ethyl-	112	C8H16	001678-91-7	72
3		Ethanone, 1-(1-methylcvclopentyl)-	126	C8H14O	013388-93-7	59
4		Cvclohexane, (1-methylethyl)-	126	C9H18	000696-29-7	58
5		Oxalic acid, cyclohexyl nonyl ester	298	C17H30O4	1000309-31-1	53



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_N\DATA\VN050219\
Data File : VN055367.D
Acq On : 2 May 2019 23:27
Operator : JC/SP
Sample : K2658-03 10X
Misc : 6.49g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 36 Sample Multiplier: 1

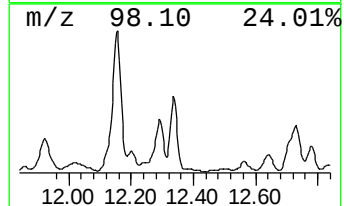
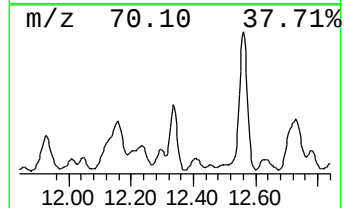
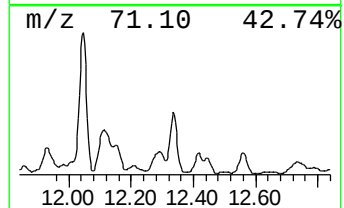
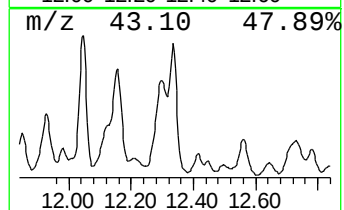
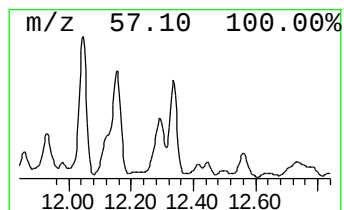
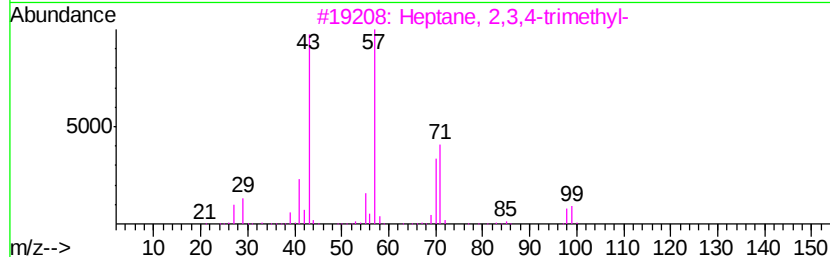
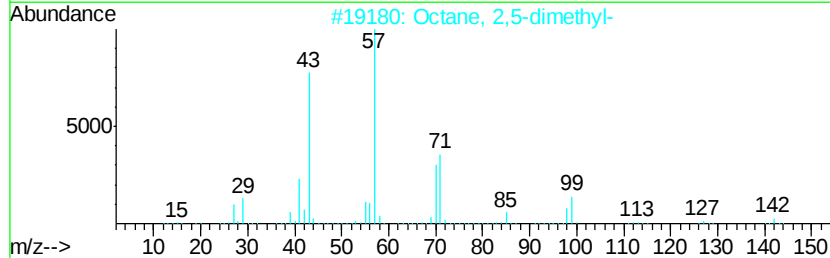
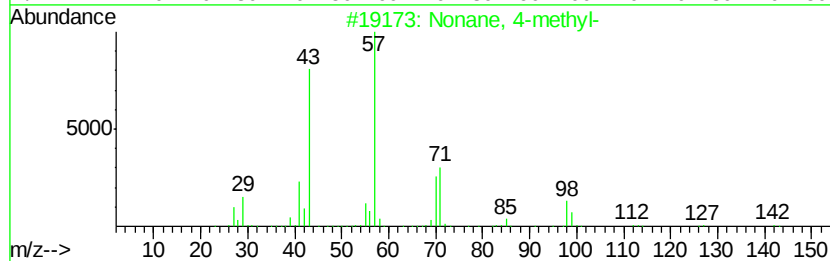
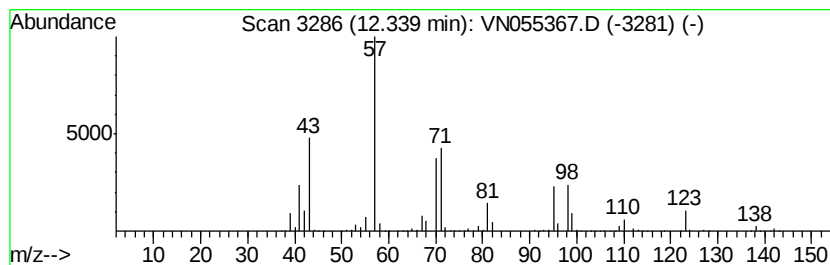
Instrument :
MSVOA_N
ClientSampleId :
EP1-SB-E6(14-17)

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N042919W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.		
12.34	188.26 ug/l	7302570	Chlorobenzene-d5	11.41		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonane, 4-methyl-	142	C10H22	017301-94-9	58	
2	Octane, 2,5-dimethyl-	142	C10H22	015869-89-3	50	
3	Heptane, 2,3,4-trimethyl-	142	C10H22	052896-95-4	50	
4	Pentane, 2,2,3,3-tetramethyl-	128	C9H20	007154-79-2	47	
5	Octane, 2,7-dimethyl-	142	C10H22	001072-16-8	43	



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN050219\
 Data File : VN055367.D
 Acq On : 2 May 2019 23:27
 Operator : JC/SP
 Sample : K2658-03 10X
 Misc : 6.49g/5mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 36 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 EP1-SB-E6(14-17)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N042919W.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
Cyclohexane, 1,1,...	11.00	140.3	ug/l	5444240	3	11.41	1939510	50.0
Heptane, 2,3-dime...	11.12	83.5	ug/l	3237890	3	11.41	1939510	50.0
Octane, 4-methyl-	11.20	200.0	ug/l	7756650	3	11.41	1939510	50.0
Octane, 3-methyl-	11.30	185.4	ug/l	7190430	3	11.41	1939510	50.0
Cyclohexane, 1-et...	11.70	123.7	ug/l	4796430	3	11.41	1939510	50.0
Cyclohexane, 1-et...	11.92	325.4	ug/l	12624300	3	11.41	1939510	50.0
Nonane, 3-methyl-	12.05	172.9	ug/l	6708150	3	11.41	1939510	50.0
1H-Indene, octahy...	12.12	179.8	ug/l	6976470	3	11.41	1939510	50.0
Cyclohexane, propyl-	12.17	450.6	ug/l	17478600	3	11.41	1939510	50.0
Nonane, 4-methyl-	12.34	188.3	ug/l	7302570	3	11.41	1939510	50.0