

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN090718\
 Data File : VN051055.D
 Acq On : 7 Sep 2018 15:50
 Operator : MD\SY
 Sample : J4693-09 5X
 Misc : 5.82g/5mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 EP1-MW-C(10-15)

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\82N082118W.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	1787	1810	1821	rBV2	466242	1188310	1.87%	0.168%
2	7.667	1821	1833	1850	rVB	756978	1794915	2.82%	0.253%
3	8.027	1928	1945	1964	rBV	458886	1052800	1.65%	0.148%
4	8.587	2102	2119	2149	rBV	1041447	2158641	3.39%	0.304%
5	9.082	2245	2273	2286	rBV	798856	1862196	2.93%	0.263%
6	10.088	2572	2586	2615	rVB3	3344945	7504950	11.79%	1.058%
7	10.258	2630	2639	2661	rVB4	376029	1012085	1.59%	0.143%
8	10.432	2661	2693	2709	rBV	1187176	2604818	4.09%	0.367%
9	10.532	2709	2724	2732	rBV	633310	1317530	2.07%	0.186%
10	10.628	2746	2754	2763	rVB	596542	960835	1.51%	0.135%
11	10.718	2772	2782	2794	rVB	1805843	3039019	4.78%	0.429%
12	10.821	2800	2814	2827	rBV	1465646	3098386	4.87%	0.437%
13	10.889	2827	2835	2842	rVV2	845685	1498563	2.36%	0.211%
14	10.953	2846	2855	2863	rVV	3565054	6195378	9.74%	0.874%
15	11.008	2863	2872	2882	rVV	4835597	8688584	13.65%	1.225%
16	11.059	2882	2888	2896	rVB	931237	1322234	2.08%	0.186%
17	11.123	2896	2908	2916	rBV3	3571110	6476511	10.18%	0.913%
18	11.165	2917	2921	2926	rVV2	905108	1334524	2.10%	0.188%
19	11.213	2927	2936	2951	rVB	4812521	9273381	14.57%	1.308%
20	11.291	2951	2960	2968	rBV	1115003	1806277	2.84%	0.255%
21	11.406	2985	2996	3004	rBV2	1601405	3146171	4.94%	0.444%
22	11.493	3015	3023	3030	rBV3	976414	1635485	2.57%	0.231%
23	11.545	3030	3039	3045	rBV	2951782	4532801	7.12%	0.639%
24	11.596	3045	3055	3063	rBV6	3578018	6951273	10.92%	0.980%
25	11.657	3063	3074	3081	rBV2	14183551	25439680	39.98%	3.588%
26	11.699	3082	3087	3097	rVB2	9582835	15143718	23.80%	2.136%
27	11.760	3097	3106	3112	rBV3	1703877	3047135	4.79%	0.430%
28	11.815	3113	3123	3128	rBV2	1893315	3424912	5.38%	0.483%
29	11.853	3128	3135	3143	rVB3	4453340	6682708	10.50%	0.942%
30	11.924	3143	3157	3170	rBV6	18263445	45824262	72.01%	6.462%
31	12.046	3188	3195	3203	rBV	15876194	22114521	34.75%	3.119%
32	12.120	3211	3218	3224	rBV3	14409872	22641796	35.58%	3.193%
33	12.168	3225	3233	3250	rVB4	26996147	53096130	83.44%	7.488%
34	12.406	3296	3307	3316	rBV8	5192875	10391647	16.33%	1.465%

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35	12.490	3317	3333	3339	rBV6	7149574	20724036	32.57%	2.923%
36	12.564	3349	3356	3372	rVB3	20898159	53048749	83.37%	7.481%
37	12.647	3373	3382	3392	rBV6	8399422	18275699	28.72%	2.577%
38	12.731	3394	3408	3417	rVV5	24035975	63631712	100.00%	8.973%
39	12.783	3418	3424	3434	rVB2	13171535	20702524	32.53%	2.920%
40	12.869	3444	3451	3458	rVV5	6660456	9353472	14.70%	1.319%
41	12.930	3459	3470	3472	rVV4	5008272	9977463	15.68%	1.407%
42	12.963	3473	3480	3494	rVB3	20999382	37676880	59.21%	5.313%
43	13.168	3533	3544	3552	rVV5	8677465	18398165	28.91%	2.595%
44	13.242	3553	3567	3588	rVB	18192966	42239378	66.38%	5.957%
45	13.512	3647	3651	3669	rVB2	6750880	15292670	24.03%	2.157%
46	13.612	3670	3682	3689	rBV2	5112366	10696636	16.81%	1.508%
47	13.663	3689	3698	3708	rVV3	17549757	32429619	50.96%	4.573%
48	13.712	3709	3713	3721	rVB2	2865353	3587929	5.64%	0.506%
49	13.889	3761	3768	3777	rVB	11919204	18363460	28.86%	2.590%
50	13.991	3792	3800	3810	rVB5	6042607	10349919	16.27%	1.460%
51	14.110	3832	3837	3840	rBV4	899626	1068259	1.68%	0.151%
52	14.178	3848	3858	3864	rBV6	5035902	10944605	17.20%	1.543%
53	14.294	3886	3894	3899	rBV2	1930419	3051952	4.80%	0.430%
54	14.332	3900	3906	3913	rVB2	2596806	3674990	5.78%	0.518%
55	14.528	3962	3967	3974	rVB3	690964	875017	1.38%	0.123%
56	14.583	3974	3984	3996	rVV2	5625877	10521492	16.53%	1.484%
57	14.647	3996	4004	4015	rVB3	1805344	3094260	4.86%	0.436%
58	14.850	4062	4067	4074	rVB3	896517	1107149	1.74%	0.156%
59	14.953	4093	4099	4111	rVB4	938528	1761810	2.77%	0.248%

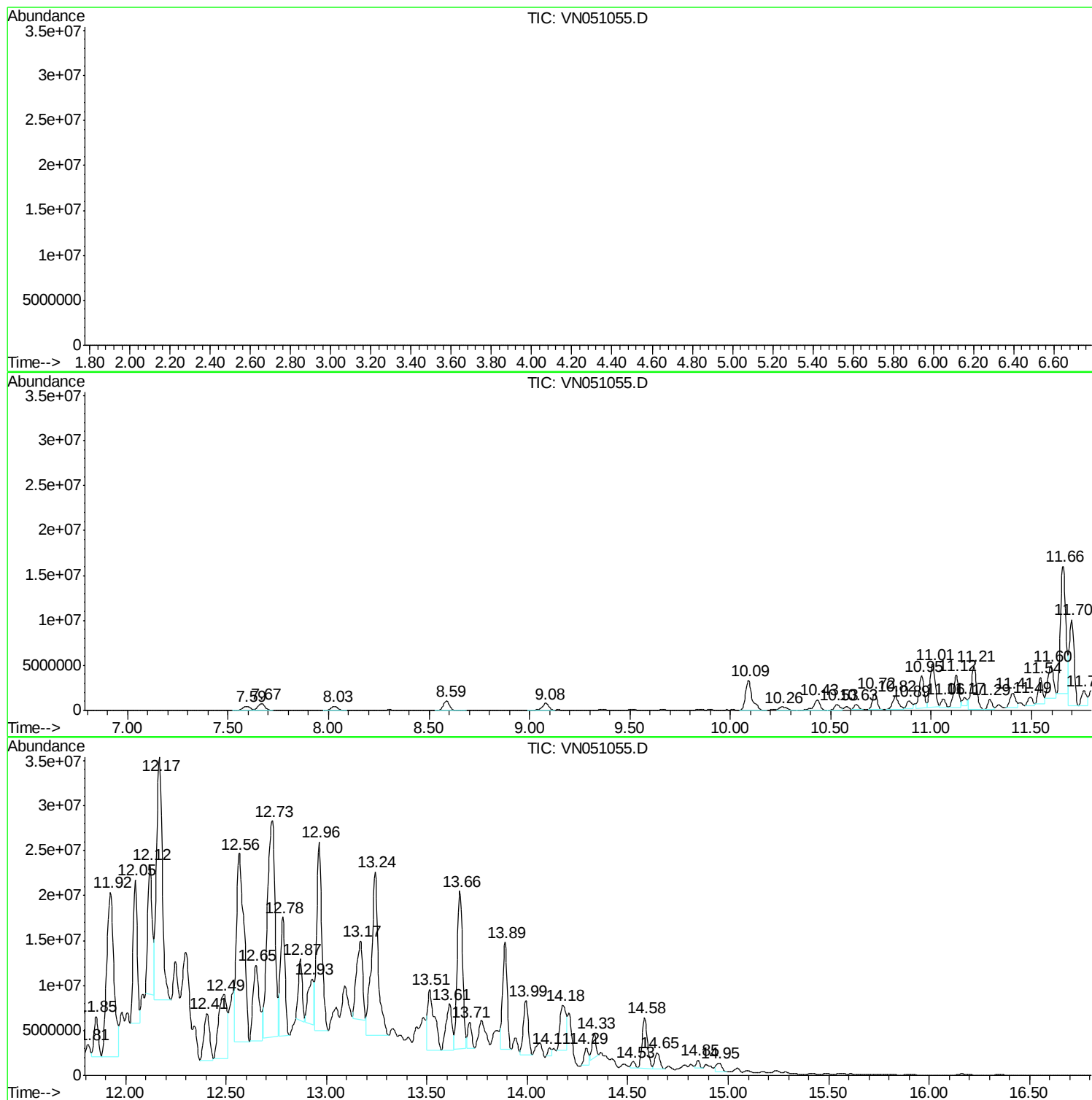
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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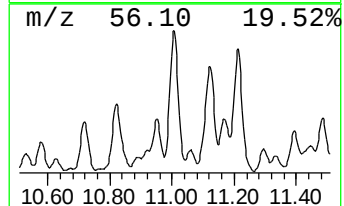
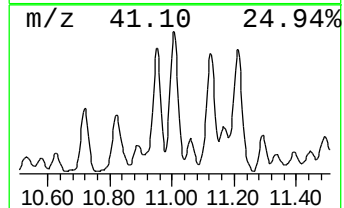
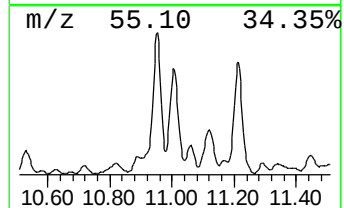
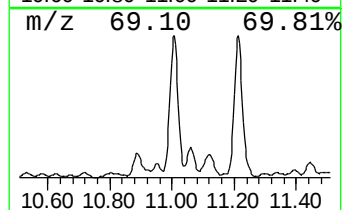
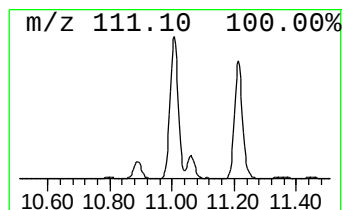
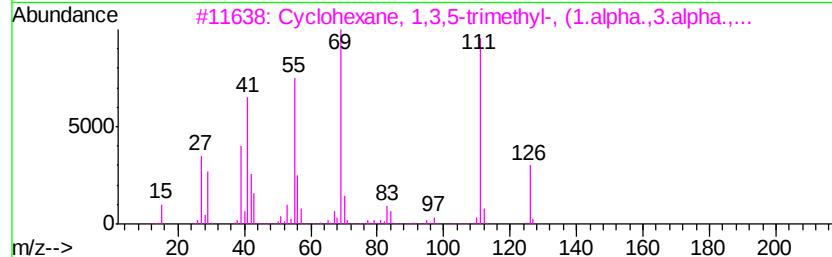
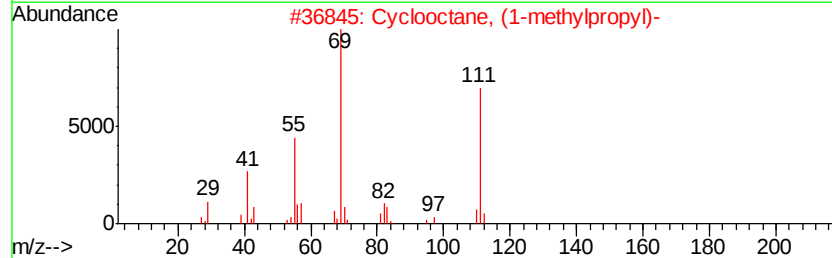
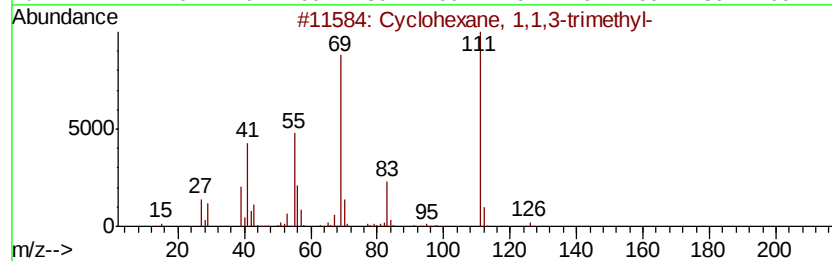
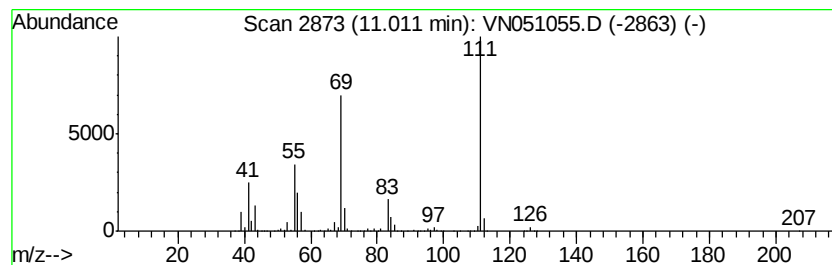
Instrument :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N082118W.M
Quant Title : SW846 8260

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.	
11.01	138.08 ug/l	8688580	Chlorobenzene-d5	11.41	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cvclohexane, 1,1,3-trimethyl-	126	C9H18	003073-66-3	95
2	Cyclooctane, (1-methylpropyl)-	168	C12H24	016538-89-9	64
3	Cvclohexane, 1,3,5-trimethyl-, (...)	126	C9H18	001795-26-2	64
4	Isocytosine	111	C4H5N3O	000108-53-2	58
5	p-Fluoroaniline	111	C6H6FN	000371-40-4	53



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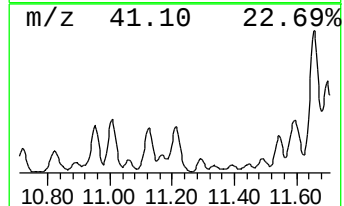
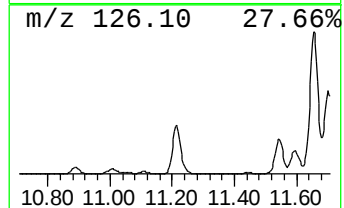
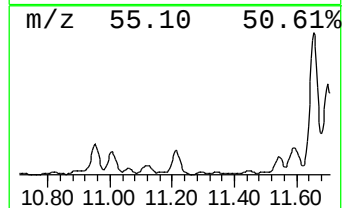
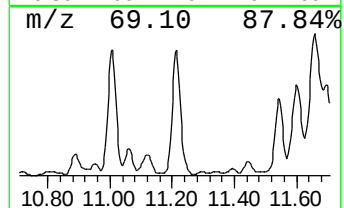
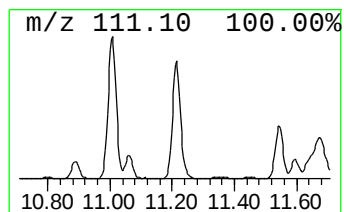
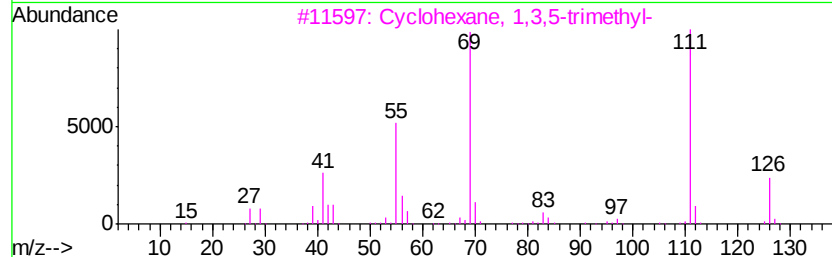
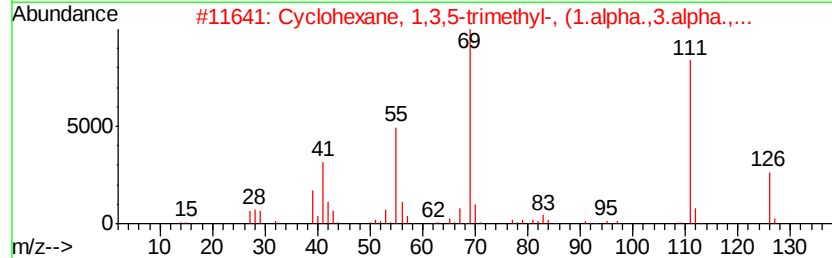
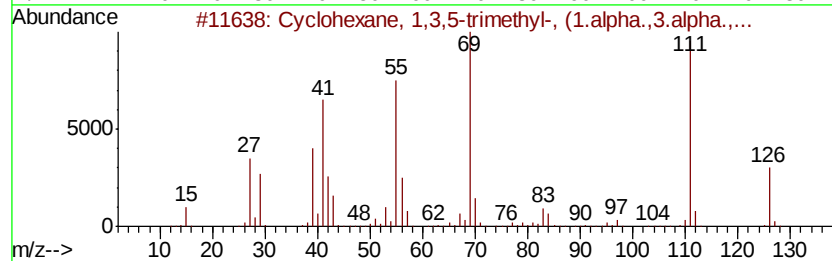
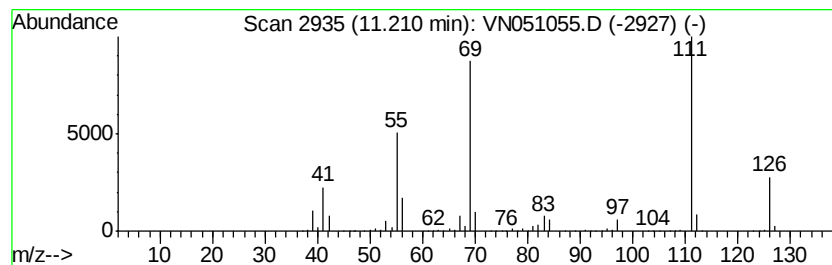
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Cyclohexane, 1,3,5-trimethy... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.21	147.38 ug/l	9273380	Chlorobenzene-d5	11.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, 1,3,5-trimethyl-, (...	126	C9H18	001795-26-2	91
2		Cyclohexane, 1,3,5-trimethyl-, (...	126	C9H18	001795-27-3	91
3		Cyclohexane, 1,3,5-trimethyl-, (...	126	C9H18	001839-63-0	90
4		Cyclohexane, 1,2,4-trimethyl-, (...	126	C9H18	007667-60-9	87
5		2-Pyrazoline, 1-isopropyl-5-methyl-	126	C7H14N2	026964-54-5	80



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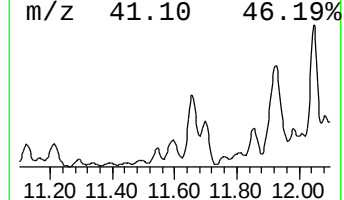
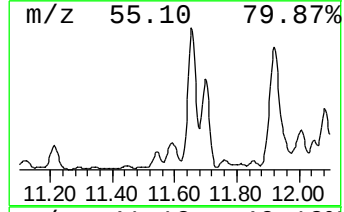
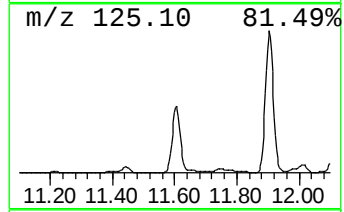
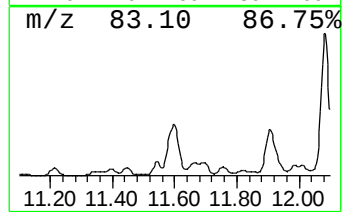
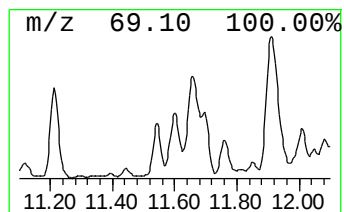
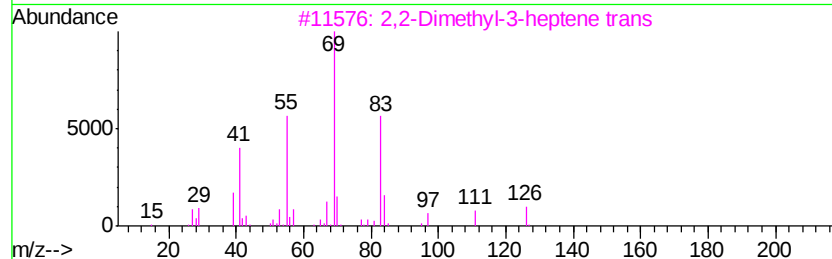
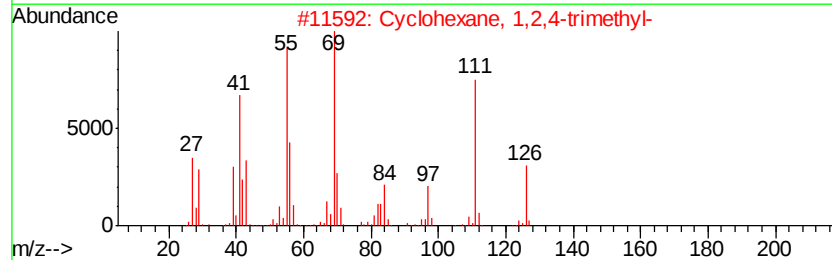
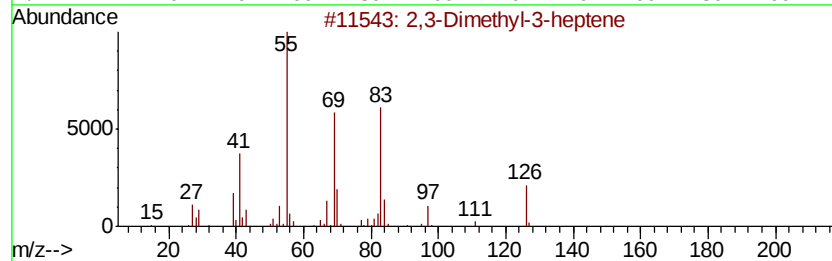
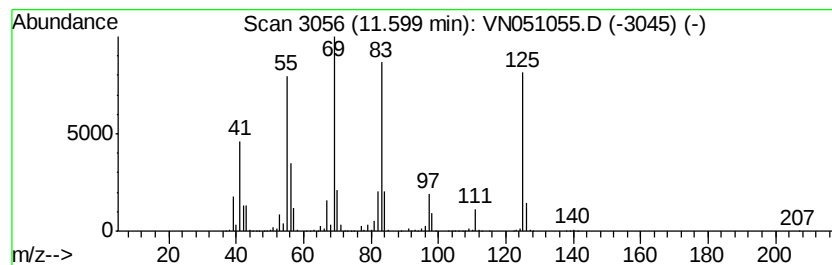
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Quant Title : SW846 8260

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

Peak Number 3 2,3-Dimethyl-3-heptene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.60	110.47 ug/l	6951270	Chlorobenzene-d5	11.41

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,3-Dimethyl-3-heptene		126	C9H18	1000113-49-3	52
2	Cyclohexane, 1,2,4-trimethyl-		126	C9H18	002234-75-5	47
3	2,2-Dimethyl-3-heptene trans		126	C9H18	019550-75-5	30
4	Cyclopentane, 1-ethyl-1-methyl-		112	C8H16	016747-50-5	30
5	3-Hexene, 2-methyl-, (E)-		98	C7H14	000692-24-0	27



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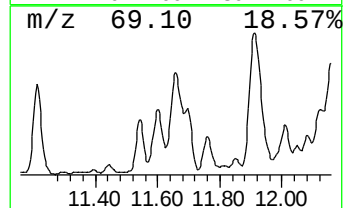
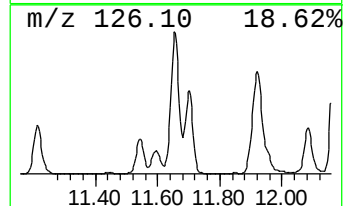
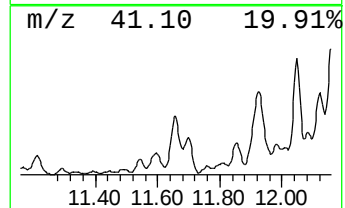
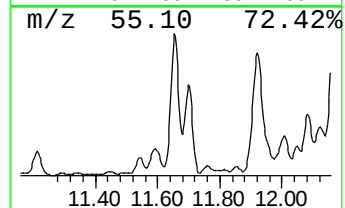
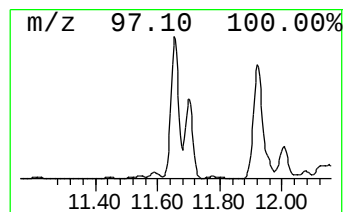
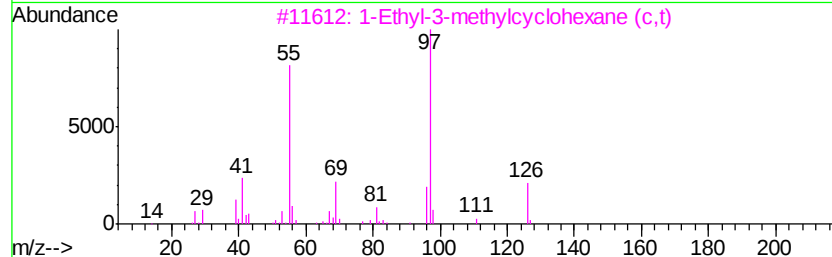
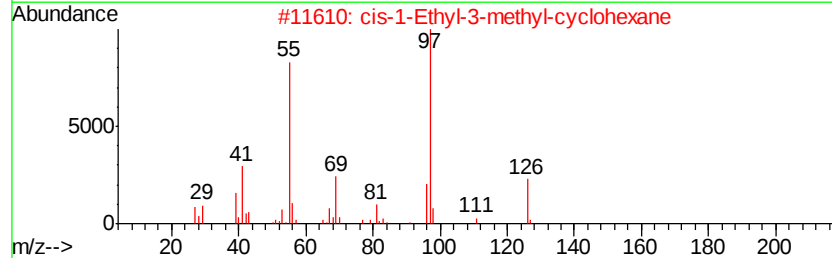
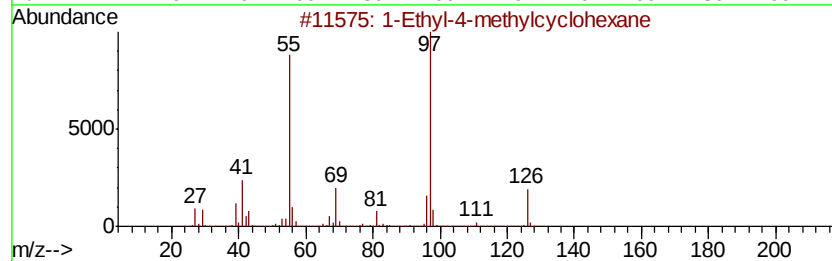
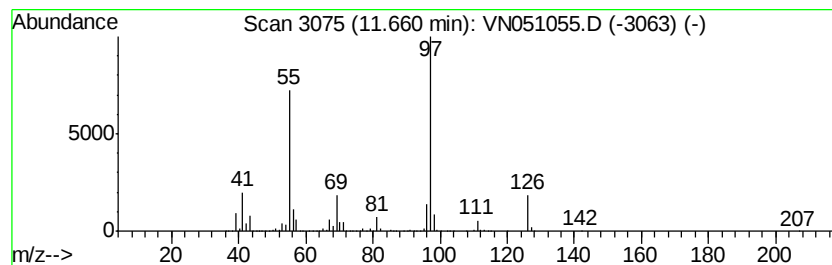
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Peak Number 4 1-Ethyl-4-methylcyclohexane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.		
11.66	404.30 ug/l	25439700	Chlorobenzene-d5	11.41		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Ethyl-4-methylcyclohexane	126	C9H18	003728-56-1	94
2		cis-1-Ethyl-3-methyl-cyclohexane	126	C9H18	019489-10-2	91
3		1-Ethyl-3-methylcyclohexane (c,t)	126	C9H18	003728-55-0	91
4		3,5-Dimethyl-3-heptene	126	C9H18	059643-68-4	87
5		Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	004926-78-7	86



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN090718\
Data File : VN051055.D
Acq On : 7 Sep 2018 15:50
Operator : MD\SY
Sample : J4693-09 5X
Misc : 5.82g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
EP1-MW-C(10-15)

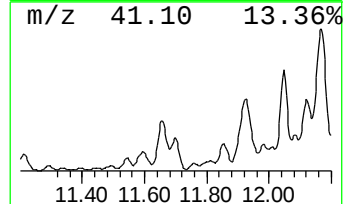
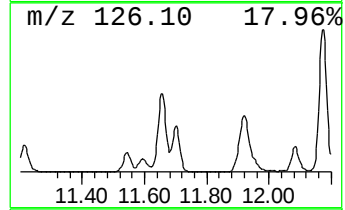
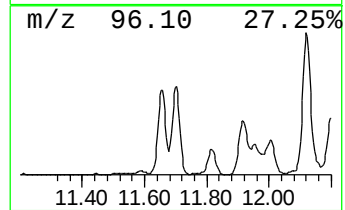
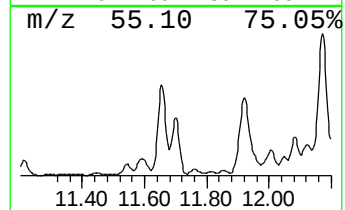
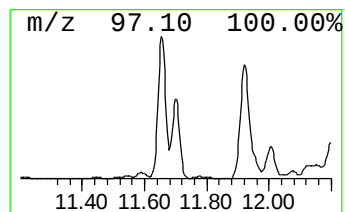
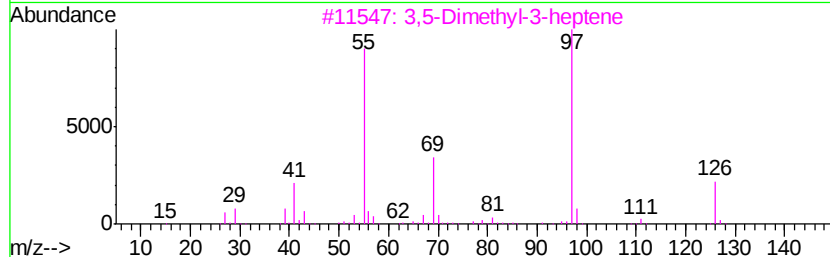
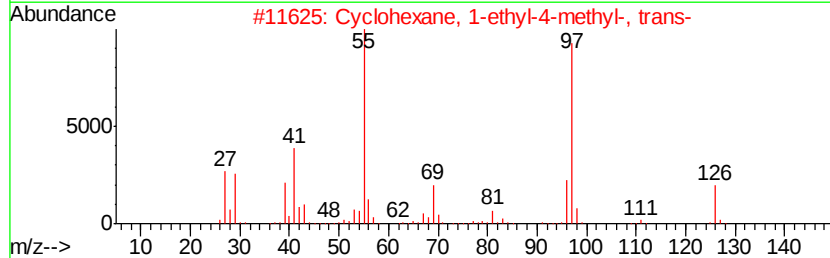
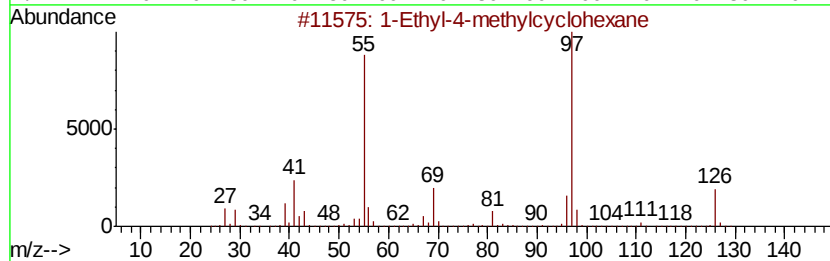
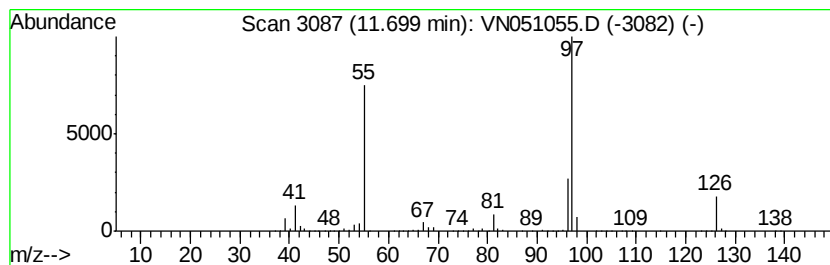
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Quant Title : SW846 8260

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

Peak Number 5 Cyclohexane, 1-ethyl-4-meth... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.70	240.67 ug/l	15143700	Chlorobenzene-d5	11.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Ethyl-4-methylcyclohexane	126	C9H18	003728-56-1	87
2		Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	006236-88-0	72
3		3,5-Dimethyl-3-heptene	126	C9H18	059643-68-4	72
4		Cyclohexane, 1-ethyl-1-methyl-	126	C9H18	004926-90-3	72
5		Cyclohexane, 1-bromo-4-methyl-	176	C7H13Br	006294-40-2	64



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_N\DATA\VN090718\
Data File : VN051055.D
Acq On : 7 Sep 2018 15:50
Operator : MD\SY
Sample : J4693-09 5X
Misc : 5.82g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
EP1-MW-C(10-15)

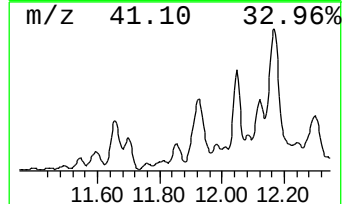
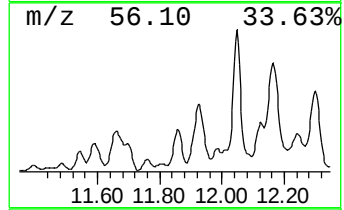
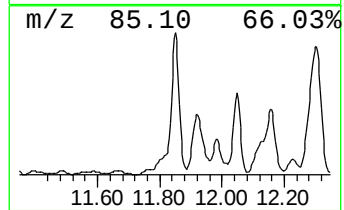
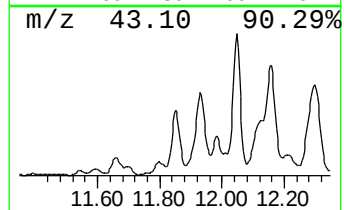
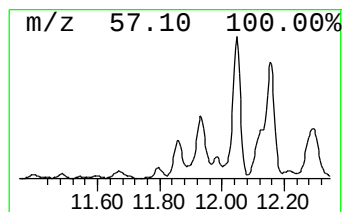
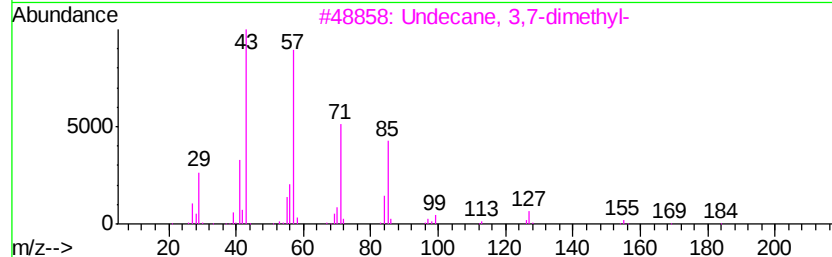
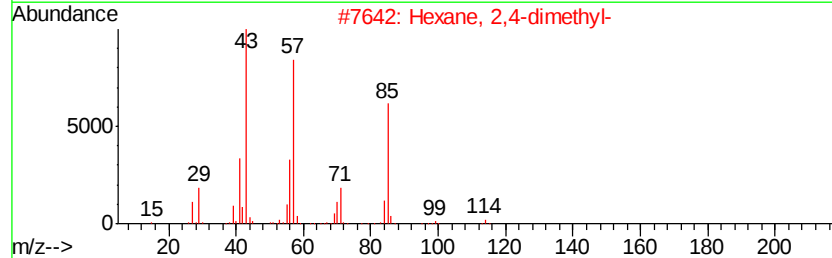
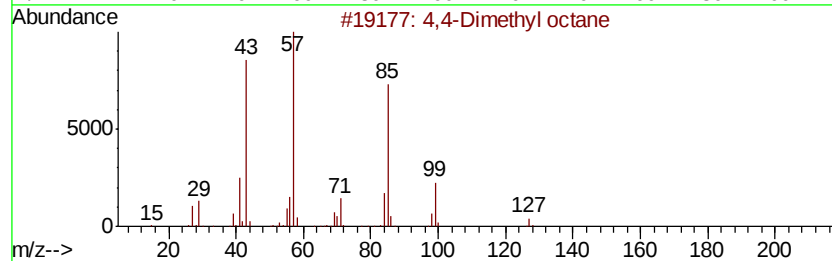
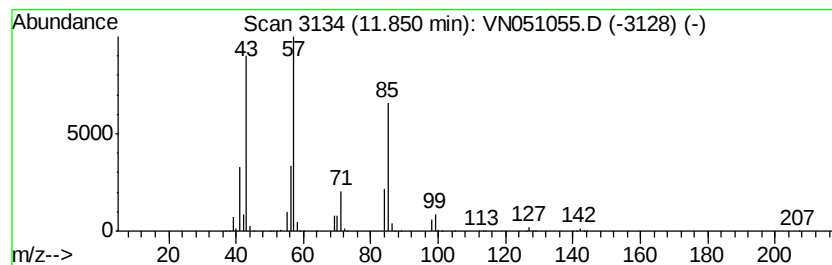
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Quant Title : SW846 8260

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

Peak Number 6 4,4-Dimethyl octane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.85	106.20 ug/l	6682710	Chlorobenzene-d5	11.41

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		4,4-Dimethyl octane	142	C10H22	015869-95-1	64
2		Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	59
3		Undecane, 3,7-dimethyl-	184	C13H28	017301-29-0	50
4		Hexane, 1,1'-oxybis-	186	C12H26O	000112-58-3	50
5		Hexane, 2,3,3-trimethyl-	128	C9H20	016747-28-7	50



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA N\DATA\VN090718\
Data File : VN051055.D
Acq On : 7 Sep 2018 15:50
Operator : MD\SY
Sample : J4693-09 5X
Misc : 5.82g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

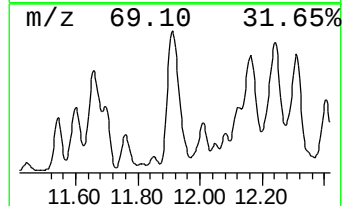
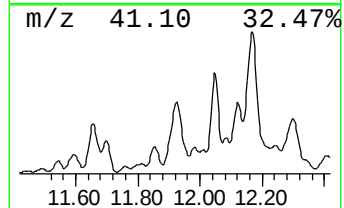
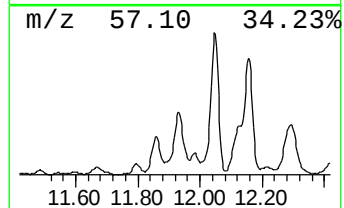
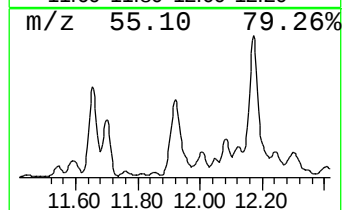
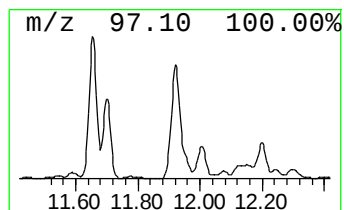
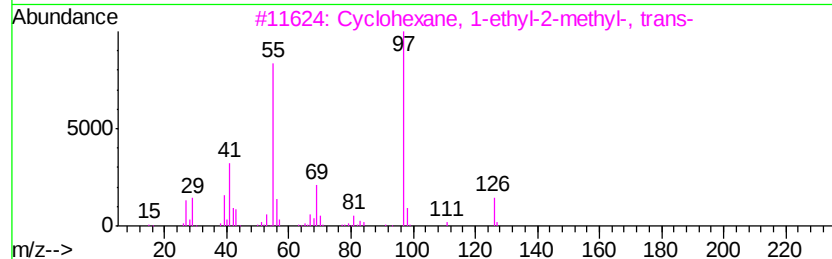
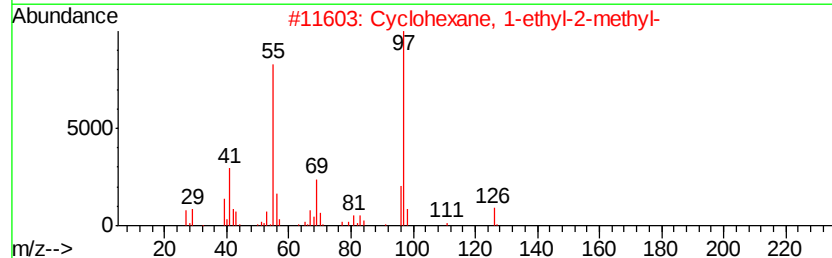
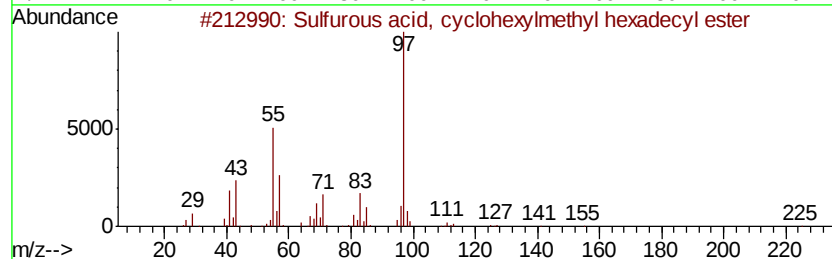
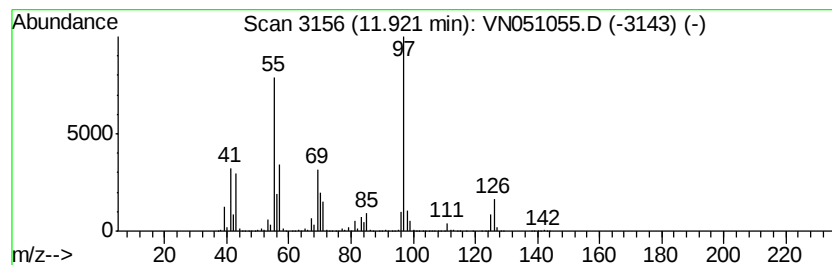
Instrument :
MSVOA_N
ClientSampleId :
EP1-MW-C(10-15)

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N082118W.M
Quant Title : SW846 8260

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

Peak Number 7 Sulfurous acid, cyclohexylm... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.		
11.92	728.25 ug/l	45824300	Chlorobenzene-d5	11.41		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Sulfurous acid, cvclohexylmethvl...	402	C23H46O3S	1000309-22-4	59
2		Cyclohexane, 1-ethyl-2-methyl-	126	C9H18	003728-54-9	58
3		Cyclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-78-8	52
4		Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	006236-88-0	52
5		Cyclohexane, 1,3-dimethyl-	112	C8H16	000591-21-9	50



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN090718\
Data File : VN051055.D
Acq On : 7 Sep 2018 15:50
Operator : MD\SY
Sample : J4693-09 5X
Misc : 5.82g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
EP1-MW-C(10-15)

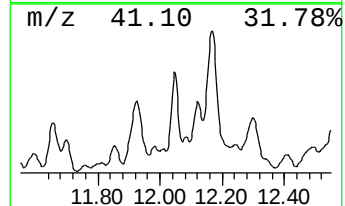
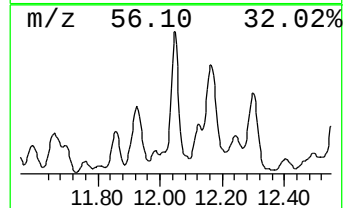
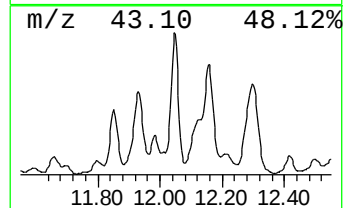
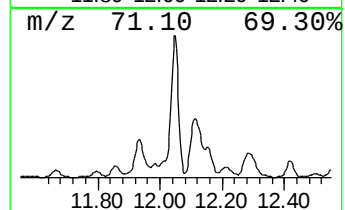
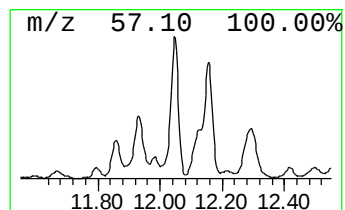
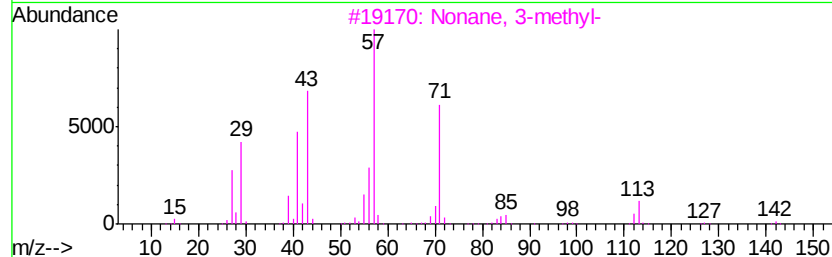
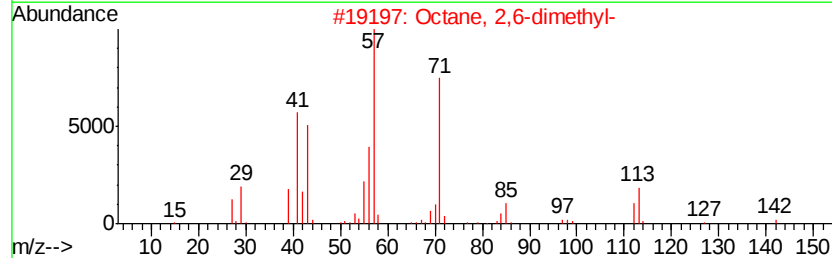
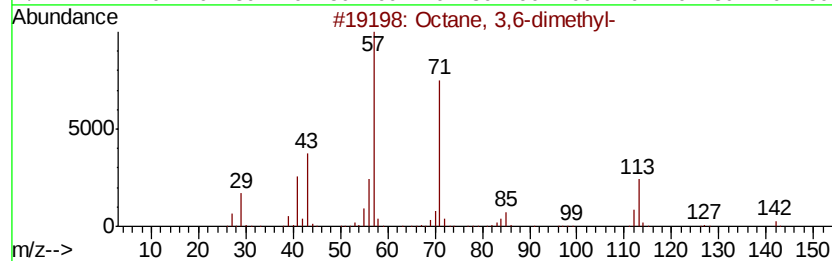
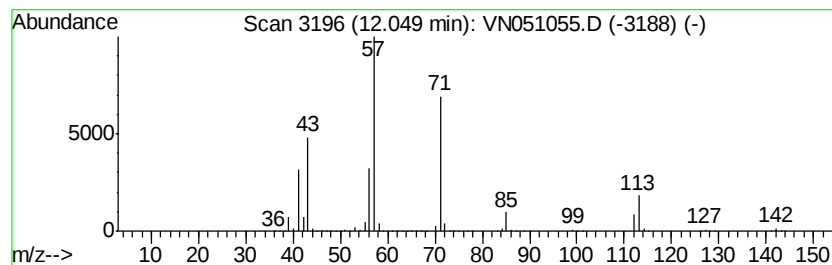
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N082118W.M
Quant Title : SW846 8260

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

Peak Number 8 Octane, 3,6-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.05	351.45 ug/l	22114500	Chlorobenzene-d5	11.41

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	91
2		Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	91
3		Nonane, 3-methyl-	142	C10H22	005911-04-6	90
4		Undecane, 6,6-dimethyl-	184	C13H28	017312-76-4	64
5		Sulfurous acid, 2-ethylhexyl hex...	418	C24H50O3S	1000309-19-9	64



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_N\DATA\VN090718\
Data File : VN051055.D
Acq On : 7 Sep 2018 15:50
Operator : MD\SY
Sample : J4693-09 5X
Misc : 5.82g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
EP1-MW-C(10-15)

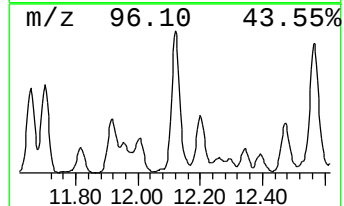
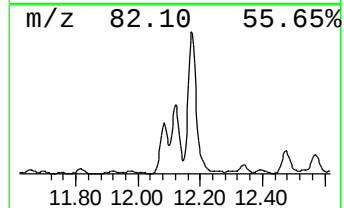
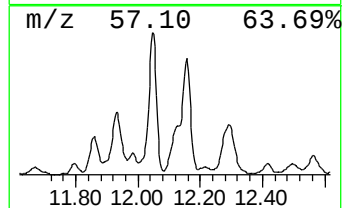
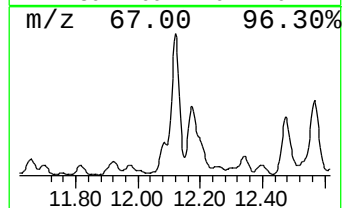
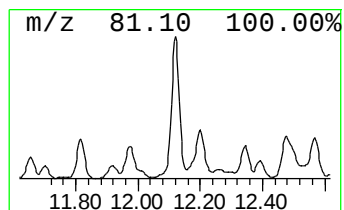
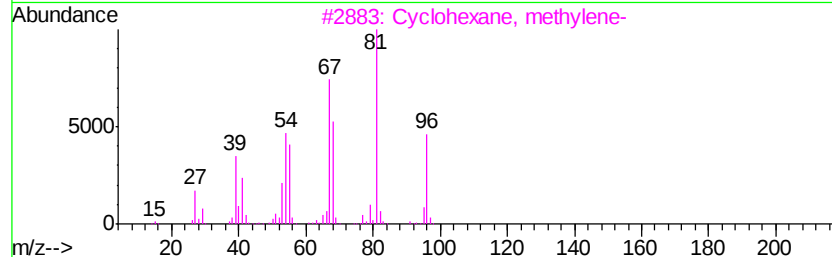
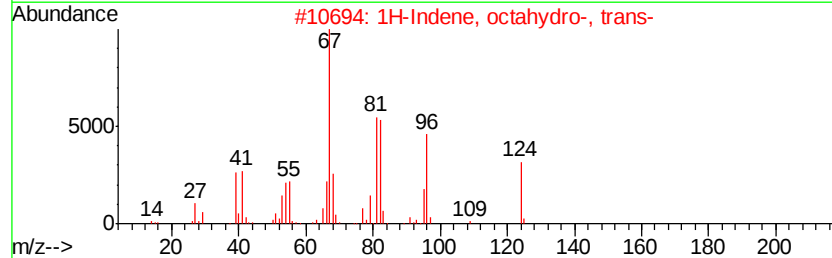
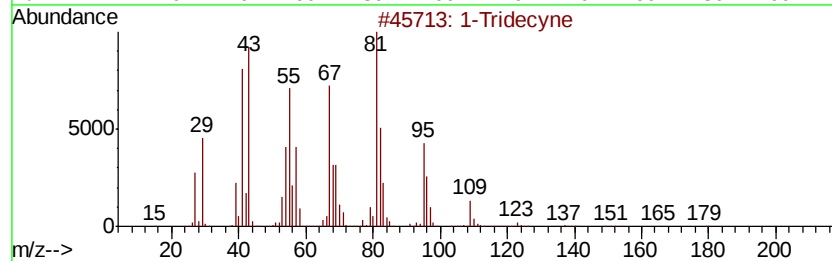
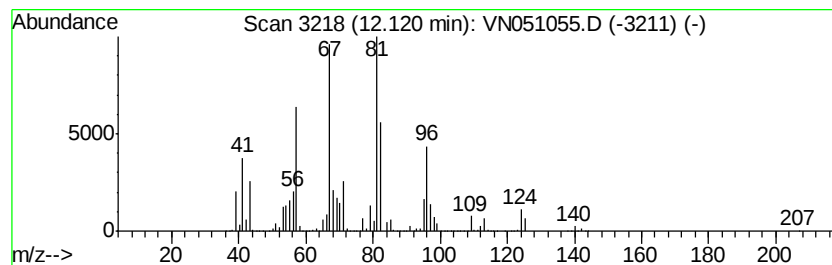
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Quant Title : SW846 8260

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

Peak Number 9 1-Tridecyne Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.12	359.83 ug/l	22641800	Chlorobenzene-d5	11.41

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tridecyne		180	C13H24	026186-02-7	59
2	1H-Indene, octahydro-, trans-		124	C9H16	003296-50-2	58
3	Cyclohexane, methylene-		96	C7H12	001192-37-6	52
4	Cyclopentane, 1,3-dimethyl-2-(1-...		138	C10H18	061142-31-2	43
5	Cyclohexene, 1-methyl-		96	C7H12	000591-49-1	38



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_N\DATA\VN090718\
Data File : VN051055.D
Acq On : 7 Sep 2018 15:50
Operator : MD\SY
Sample : J4693-09 5X
Misc : 5.82g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

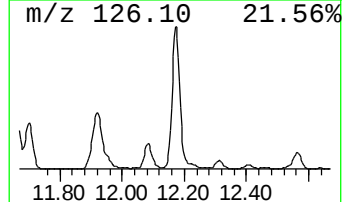
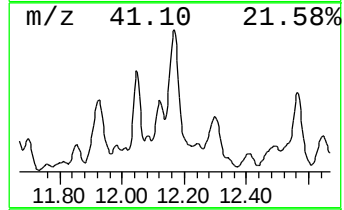
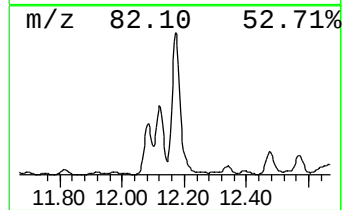
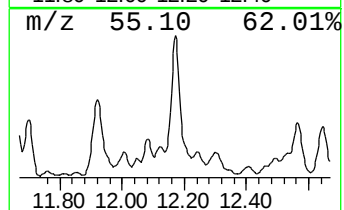
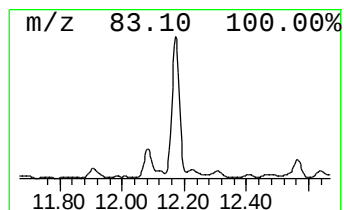
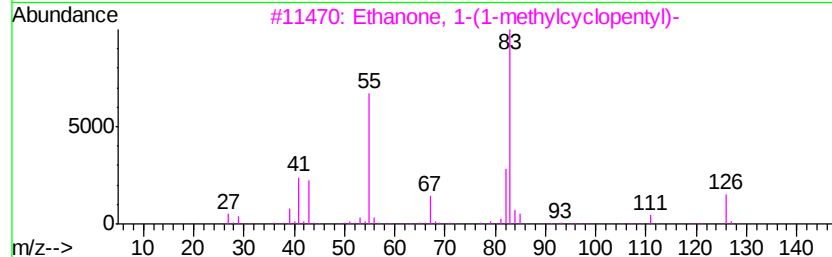
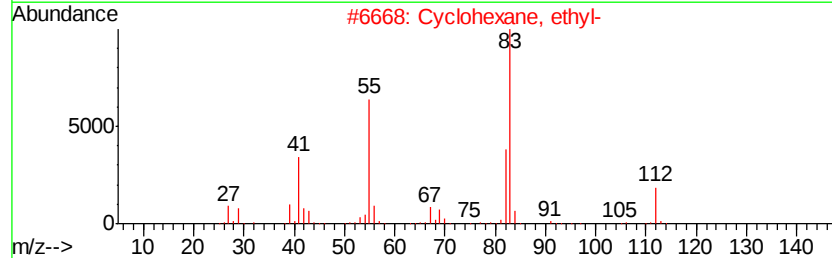
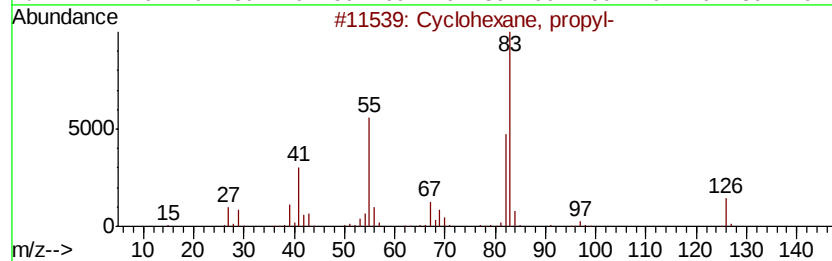
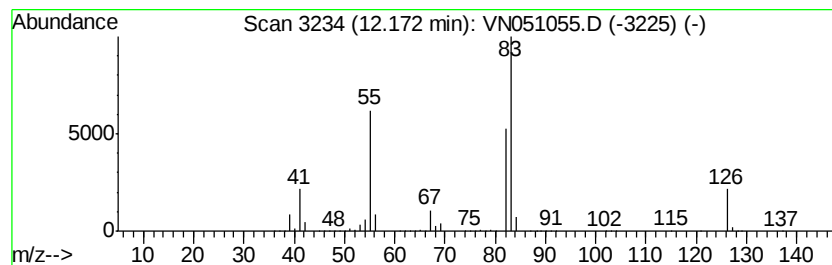
Instrument :
MSVOA_N
ClientSampleID :
EP1-MW-C(10-15)

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N082118W.M
Quant Title : SW846 8260

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

Peak Number 10 Cyclohexane, propyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.		
12.17	843.82 ug/l	53096100	Chlorobenzene-d5	11.41		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cvclohexane, propyl-	126	C9H18	001678-92-8	78
2		Cvclohexane, ethyl-	112	C8H16	001678-91-7	59
3		Ethanone, 1-(1-methylcyclopentyl)-	126	C8H14O	013388-93-7	59
4		Oxalic acid, cyclohexyl undecyl ...	326	C19H34O4	1000309-31-3	53
5		Cyclopentane, 1-ethyl-1-methyl-	112	C8H16	016747-50-5	53



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN090718\
Data File : VN051055.D
Acq On : 7 Sep 2018 15:50
Operator : MD\SY
Sample : J4693-09 5X
Misc : 5.82g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
EP1-MW-C(10-15)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N082118W.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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Cyclohexane, 1,3,...	11.21	147.4	ug/l	9273380	3	11.41	3146170	50.0
2,3-Dimethyl-3-he...	11.60	110.5	ug/l	6951270	3	11.41	3146170	50.0
1-Ethyl-4-methylc...	11.66	404.3	ug/l	25439700	3	11.41	3146170	50.0
Cyclohexane, 1-et...	11.70	240.7	ug/l	15143700	3	11.41	3146170	50.0
4,4-Dimethyl octane	11.85	106.2	ug/l	6682710	3	11.41	3146170	50.0
Sulfurous acid, c...	11.92	728.3	ug/l	45824300	3	11.41	3146170	50.0
Octane, 3,6-dimet...	12.05	351.4	ug/l	22114500	3	11.41	3146170	50.0
1-Tridecyne	12.12	359.8	ug/l	22641800	3	11.41	3146170	50.0
Cyclohexane, propyl-	12.17	843.8	ug/l	53096100	3	11.41	3146170	50.0