

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN090718\
 Data File : VN051051.D
 Acq On : 7 Sep 2018 14:11
 Operator : MD\SY
 Sample : J4693-10
 Misc : 5.91µ/5mL/100µL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 EP1-MW-C(15-20)

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	7.590	1786	1809	1820	rBV	428446	1075942	1.72%	0.152%
2	7.664	1820	1832	1850	rVB	680035	1606979	2.56%	0.227%
3	8.024	1927	1944	1963	rBV	406555	950160	1.52%	0.134%
4	8.587	2101	2119	2146	rBV	932550	1930661	3.08%	0.273%
5	9.079	2246	2272	2285	rBV	585781	1374208	2.19%	0.194%
6	10.088	2571	2586	2613	rBV2	3205021	7012710	11.19%	0.992%
7	10.259	2630	2639	2659	rVB4	343738	942175	1.50%	0.133%
8	10.432	2661	2693	2709	rBV	1164051	2594627	4.14%	0.367%
9	10.532	2709	2724	2732	rBV	620409	1293282	2.06%	0.183%
10	10.625	2745	2753	2763	rVB	616906	991842	1.58%	0.140%
11	10.718	2771	2782	2794	rVB	2090379	3494890	5.58%	0.495%
12	10.821	2799	2814	2827	rBV	1374635	2950724	4.71%	0.418%
13	10.889	2827	2835	2841	rBV2	765114	1320294	2.11%	0.187%
14	10.950	2846	2854	2862	rVV	3521036	5528295	8.82%	0.782%
15	11.004	2862	2871	2882	rVB	5044034	8512618	13.58%	1.205%
16	11.059	2882	2888	2896	rVB	926435	1330957	2.12%	0.188%
17	11.123	2896	2908	2916	rBV3	4048622	7185058	11.46%	1.017%
18	11.210	2926	2935	2951	rVB	4970067	9415156	15.02%	1.332%
19	11.291	2951	2960	2967	rBV	991623	1600712	2.55%	0.227%
20	11.406	2985	2996	3004	rBV2	1497213	3062998	4.89%	0.433%
21	11.493	3014	3023	3030	rBV3	980017	1715372	2.74%	0.243%
22	11.541	3030	3038	3045	rBV	2720788	4180444	6.67%	0.592%
23	11.593	3045	3054	3063	rBV6	3051373	5796645	9.25%	0.820%
24	11.654	3063	3073	3081	rBV2	12340561	22130272	35.31%	3.132%
25	11.699	3082	3087	3097	rVB2	8180201	12436370	19.84%	1.760%
26	11.760	3097	3106	3111	rBV3	1556490	2693916	4.30%	0.381%
27	11.812	3112	3122	3127	rBV2	1689159	3180835	5.07%	0.450%
28	11.853	3128	3135	3143	rVB3	4861261	7245856	11.56%	1.025%
29	11.924	3143	3157	3169	rBV5	15745727	38794543	61.89%	5.490%
30	12.046	3187	3195	3203	rBV	18924220	26065295	41.58%	3.689%
31	12.120	3210	3218	3224	rBV2	14203406	24101649	38.45%	3.411%
32	12.165	3225	3232	3250	rVB4	22964230	46111361	73.56%	6.526%
33	12.406	3296	3307	3316	rBV7	4568996	9192174	14.66%	1.301%
34	12.490	3317	3333	3339	rBV6	6523053	18613570	29.69%	2.634%

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35	12.564	3349	3356	3372	rVB3	18225162	45082318	71.92%	6.380%
36	12.648	3372	3382	3391	rBV8	8284844	17275578	27.56%	2.445%
37	12.728	3394	3407	3417	rVV5	23582899	62682610	100.00%	8.871%
38	12.783	3418	3424	3434	rVB3	13295859	20975157	33.46%	2.968%
39	12.869	3444	3451	3458	rBV5	7229544	10629968	16.96%	1.504%
40	12.963	3473	3480	3493	rVB2	31373503	53966685	86.10%	7.637%
41	13.091	3514	3520	3530	rVV5	4603922	7379333	11.77%	1.044%
42	13.168	3532	3544	3552	rVV6	8401538	19735840	31.49%	2.793%
43	13.242	3553	3567	3588	rVB3	20184381	47949278	76.50%	6.786%
44	13.612	3671	3682	3688	rBV2	4365596	8918405	14.23%	1.262%
45	13.664	3689	3698	3708	rVV5	18794611	35370852	56.43%	5.006%
46	13.712	3709	3713	3721	rVB2	4727298	6059218	9.67%	0.857%
47	13.773	3725	3732	3744	rVB8	4036533	8794840	14.03%	1.245%
48	13.889	3761	3768	3777	rVB	12127665	18948165	30.23%	2.681%
49	13.992	3792	3800	3810	rVB5	5936509	10298692	16.43%	1.457%
50	14.175	3848	3857	3865	rBV6	7253853	15316964	24.44%	2.168%
51	14.291	3886	3893	3898	rBV2	1558586	2345683	3.74%	0.332%
52	14.332	3899	3906	3913	rVV2	3975200	5706860	9.10%	0.808%
53	14.525	3962	3966	3973	rVB4	753775	897651	1.43%	0.127%
54	14.583	3974	3984	3995	rVV2	6841746	12906990	20.59%	1.827%
55	14.644	3996	4003	4014	rVB3	2773909	4858607	7.75%	0.688%
56	14.889	4074	4079	4090	rVV4	631404	1191418	1.90%	0.169%
57	14.953	4092	4099	4110	rVB4	1101706	2184472	3.48%	0.309%
58	15.091	4137	4142	4156	rVB4	318907	720514	1.15%	0.102%

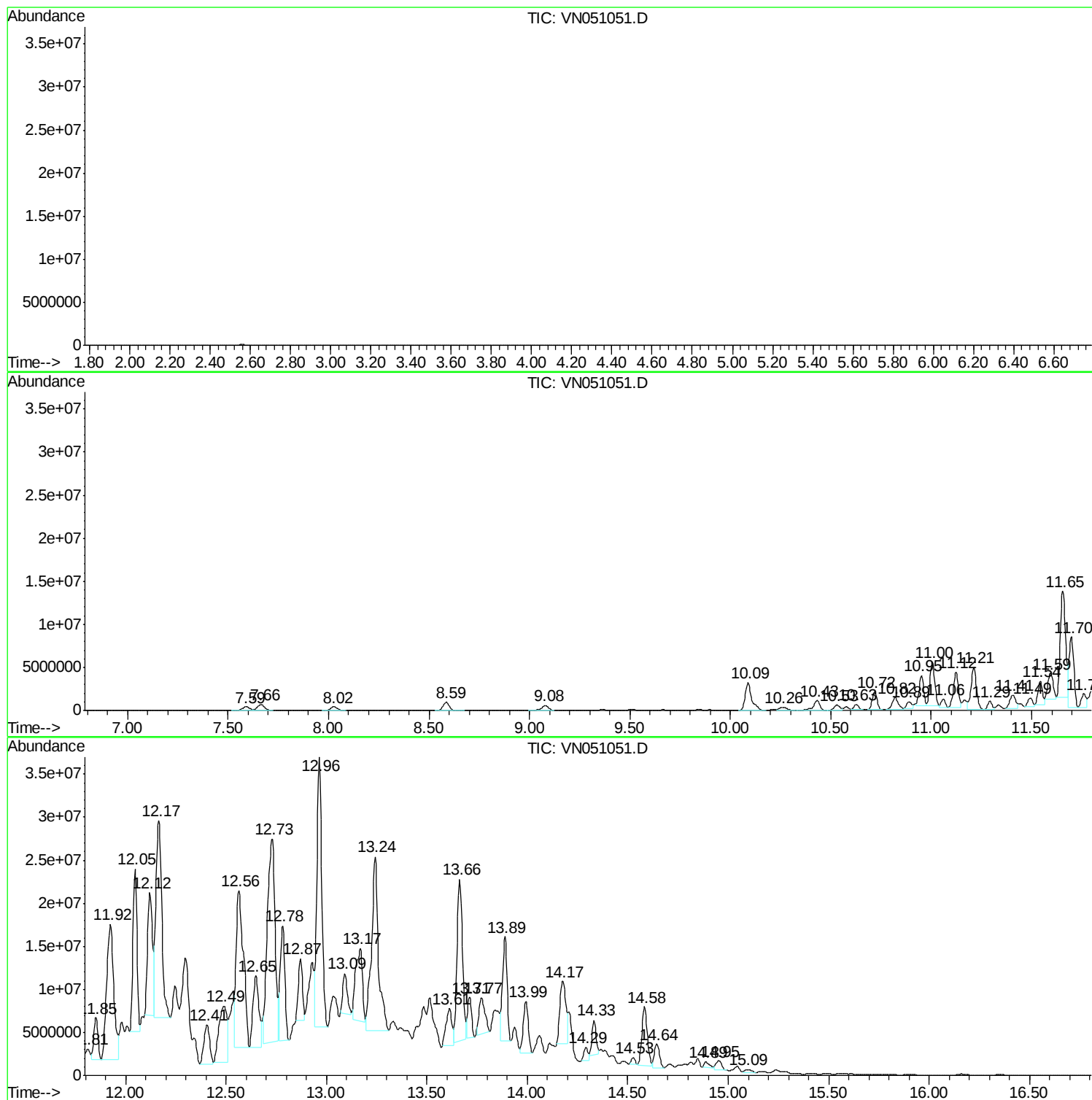
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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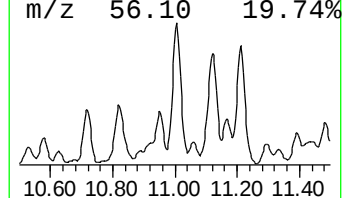
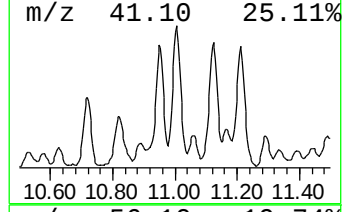
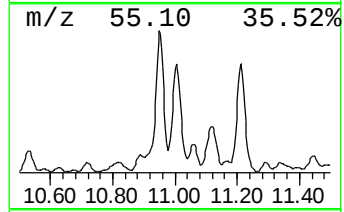
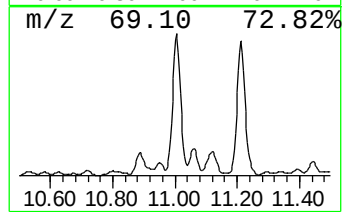
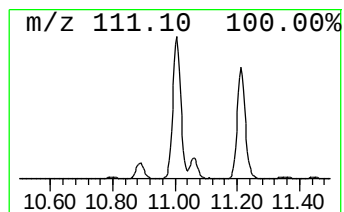
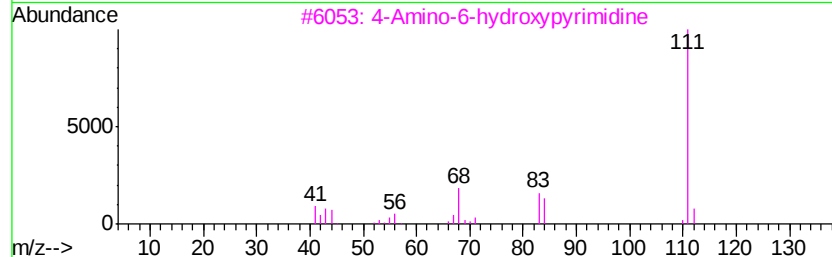
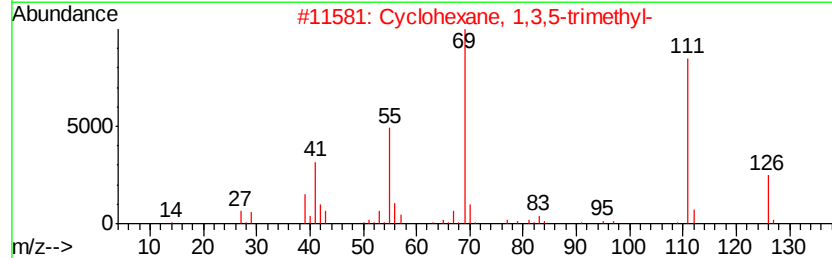
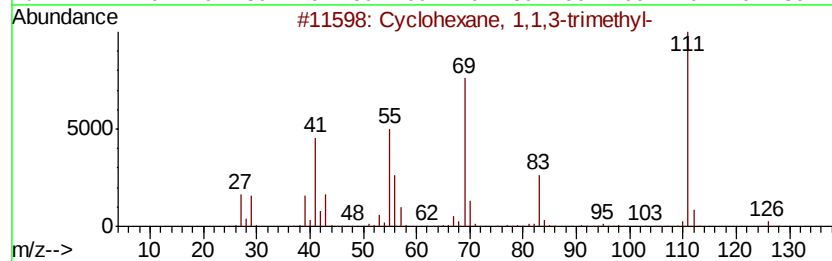
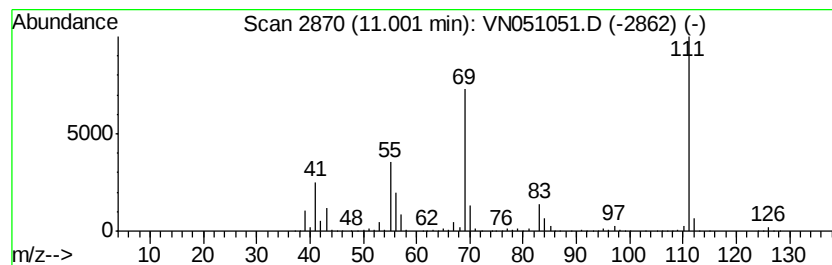
Instrument :
MSVOA_N
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N082118W.M
Quant Title : SW846 8260

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.		
11.00	138.96 ug/l	8512620	Chlorobenzene-d5	11.41		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cvclohexane, 1,1,3-trimethyl-	126	C9H18	003073-66-3	70
2		Cvclohexane, 1,3,5-trimethyl-	126	C9H18	001839-63-0	64
3		4-Amino-6-hydroxvpvrimidine	111	C4H5N3O	001193-22-2	53
4		Isocytosine	111	C4H5N3O	000108-53-2	53
5		p-Fluoroaniline	111	C6H6FN	000371-40-4	50



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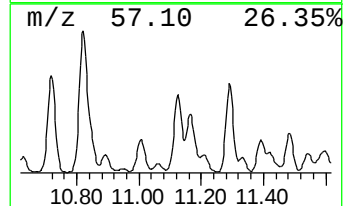
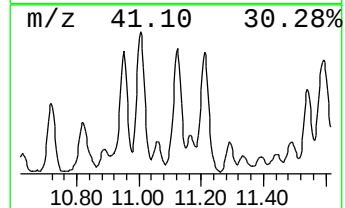
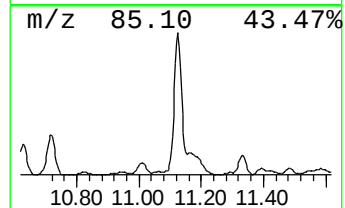
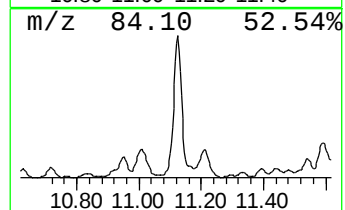
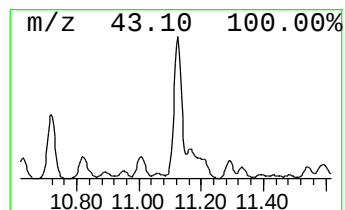
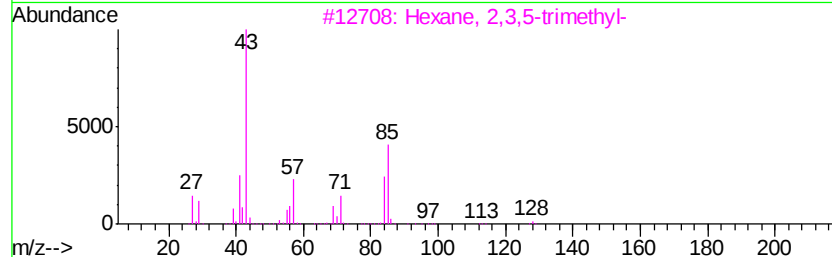
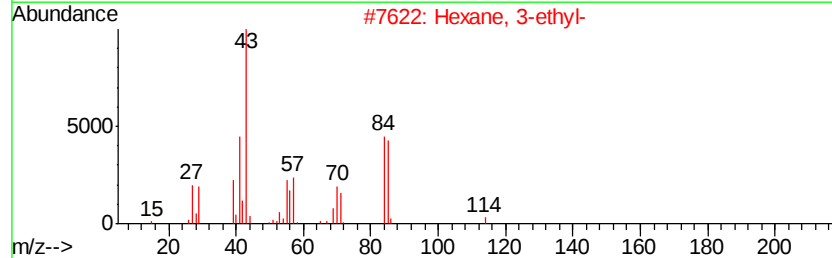
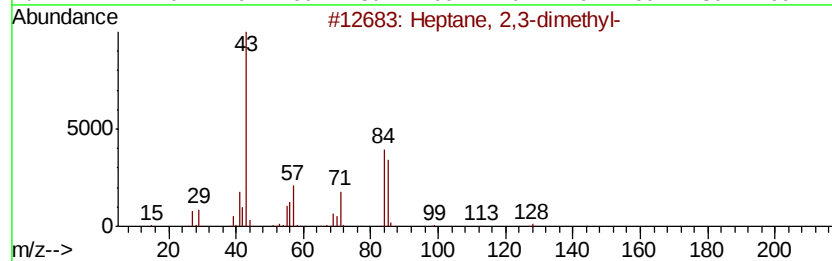
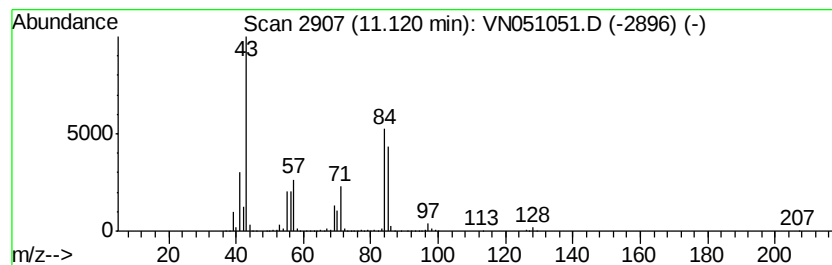
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.12	117.29 ug/l	7185060	Chlorobenzene-d5	11.41

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane, 2,3-dimethyl-	128	C9H20	003074-71-3	87	
2	Hexane, 3-ethyl-	114	C8H18	000619-99-8	83	
3	Hexane, 2,3,5-trimethyl-	128	C9H20	001069-53-0	72	
4	Decane, 5,6-dimethyl-	170	C12H26	001636-43-7	59	
5	Nonane	128	C9H20	000111-84-2	50	



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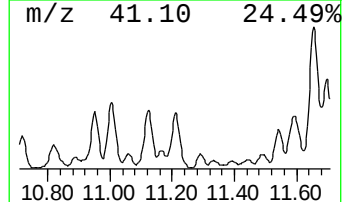
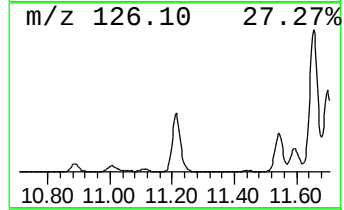
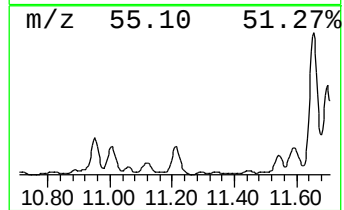
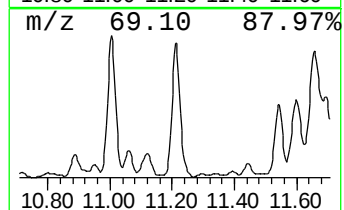
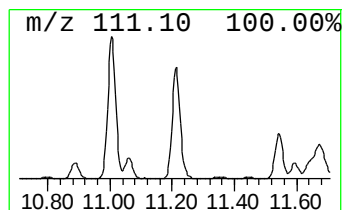
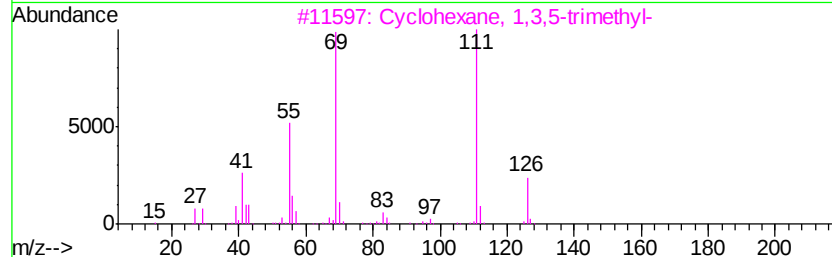
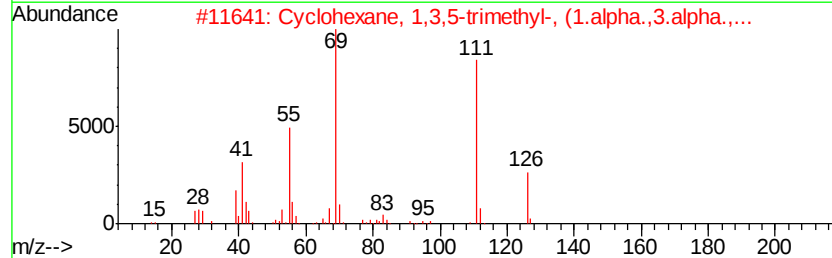
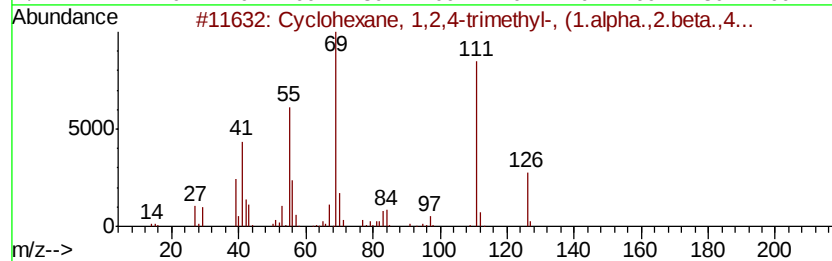
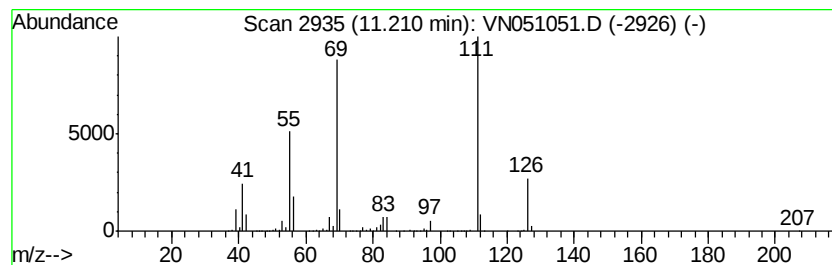
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Cyclohexane, 1,2,4-trimethy... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.21	153.69 ug/l	9415160	Chlorobenzene-d5	11.41

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



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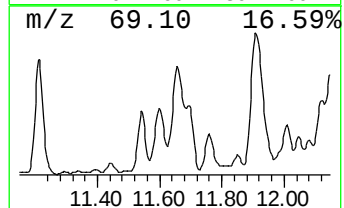
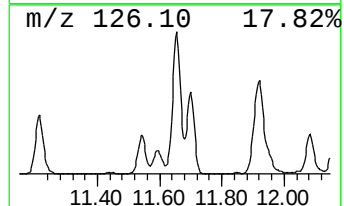
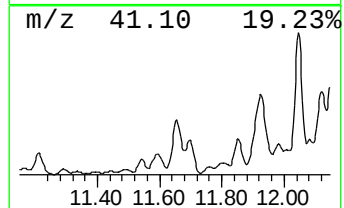
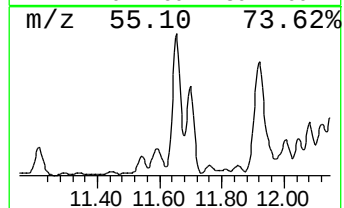
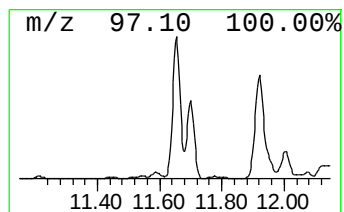
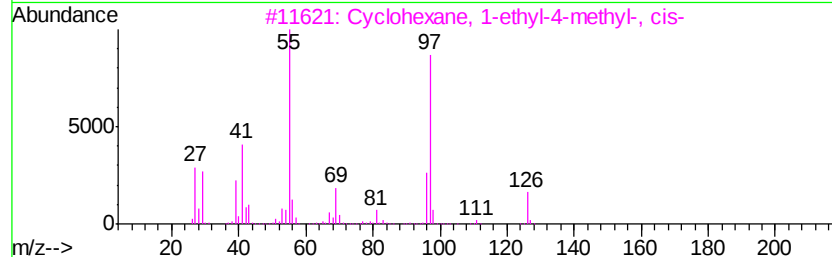
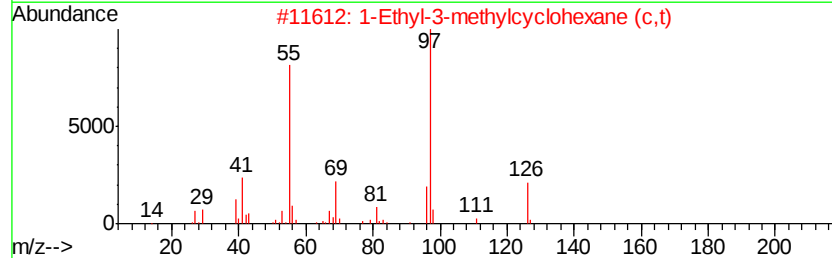
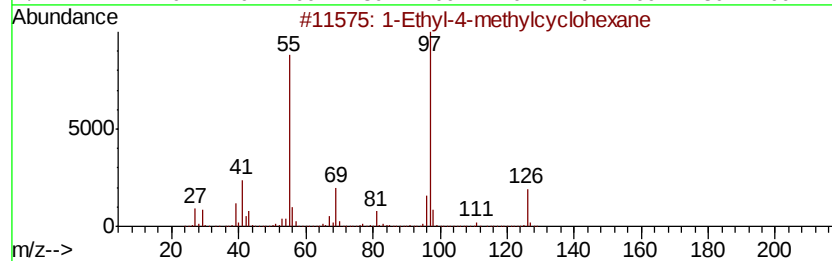
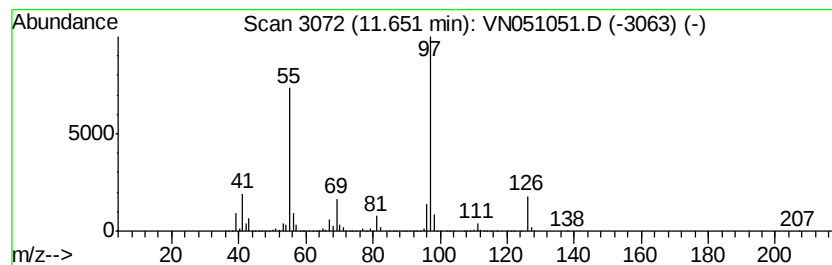
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Peak Number 4 1-Ethyl-4-methylcyclohexane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.		
11.65	361.25 ug/l	22130300	Chlorobenzene-d5	11.41		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Ethyl-4-methylcyclohexane	126	C9H18	003728-56-1	95
2		1-Ethyl-3-methylcyclohexane (c,t)	126	C9H18	003728-55-0	91
3		Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	004926-78-7	87
4		3,5-Dimethyl-3-heptene	126	C9H18	059643-68-4	87
5		1H-Pyrazole, 4,5-dihydro-3-methy...	126	C7H14N2	026964-49-8	80



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Operator : MD\SY
Sample : J4693-10
Misc : 5.91µ/5mL/100µL/5.00mL/MSVOA_N/MEOH
ALS Vial : 12 Sample Multiplier: 1

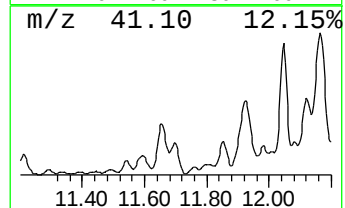
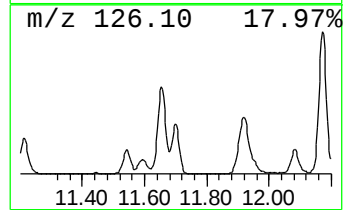
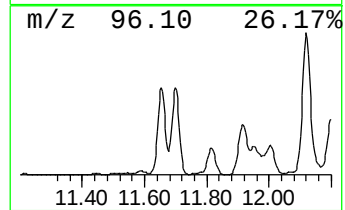
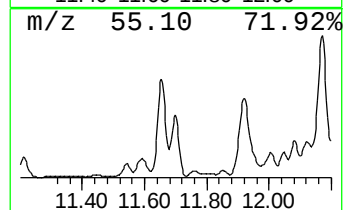
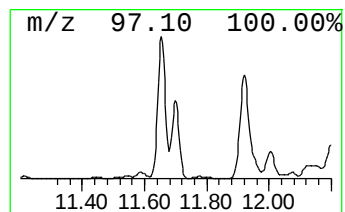
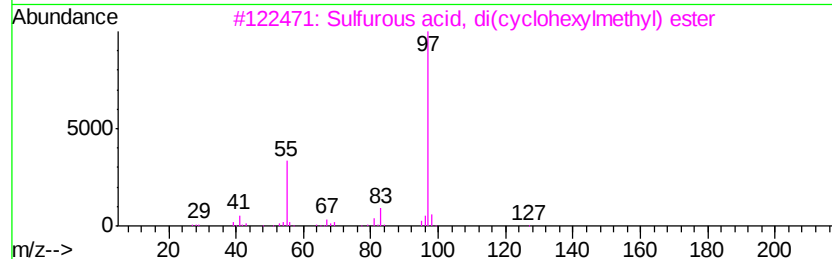
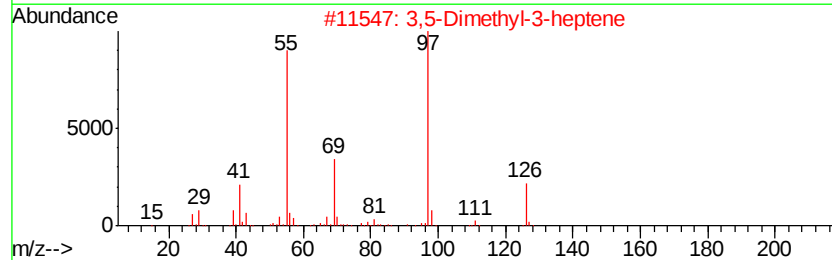
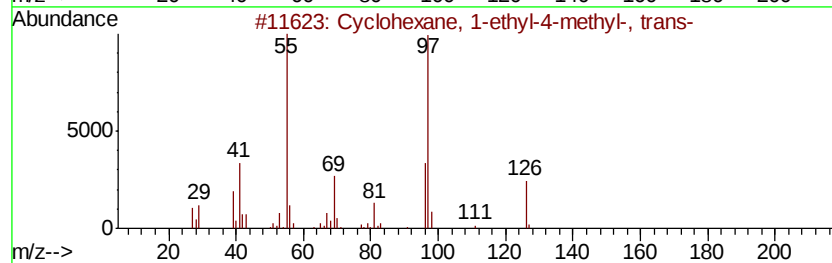
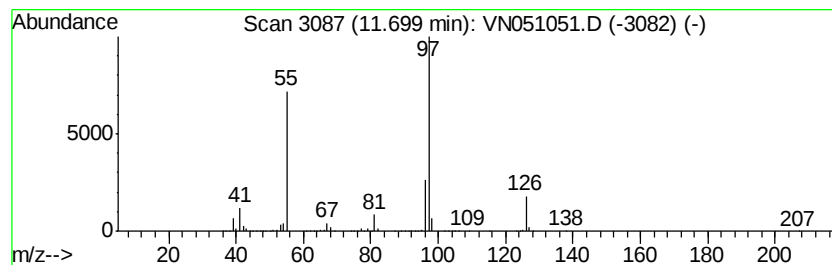
Instrument :
MSVOA_N
ClientSampleId :
EP1-MW-C(15-20)

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.70	203.01 ug/l	12436400	Chlorobenzene-d5	11.41	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	006236-88-0	78
2	3,5-Dimethyl-3-heptene	126	C9H18	059643-68-4	64
3	Sulfurous acid, di(cyclohexylmet...	274	C14H26O3S	1000309-22-7	59
4	4-Octen-3-one	126	C8H14O	014129-48-7	59
5	Oxalic acid, cyclohexylmethyl is...	270	C15H26O4	1000309-68-3	56



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN090718\
Data File : VN051051.D
Acq On : 7 Sep 2018 14:11
Operator : MD\SY
Sample : J4693-10
Misc : 5.91µ/5mL/100µL/5.00mL/MSVOA_N/MEOH
ALS Vial : 12 Sample Multiplier: 1

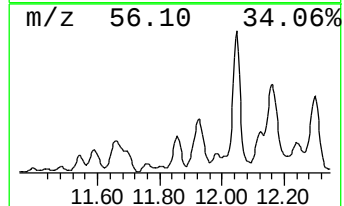
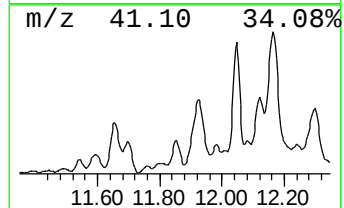
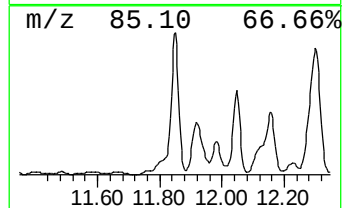
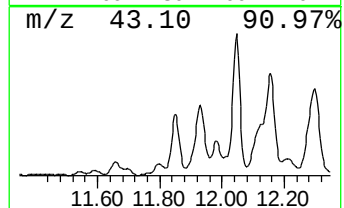
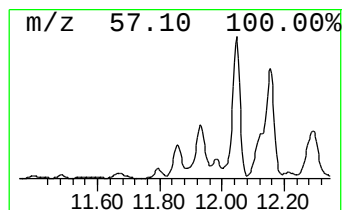
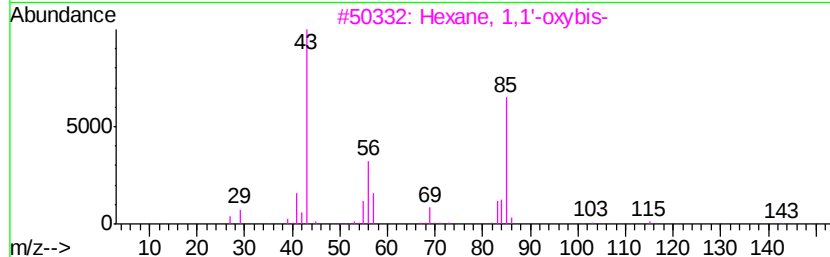
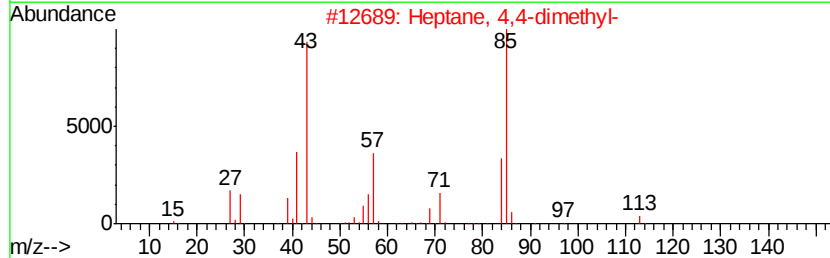
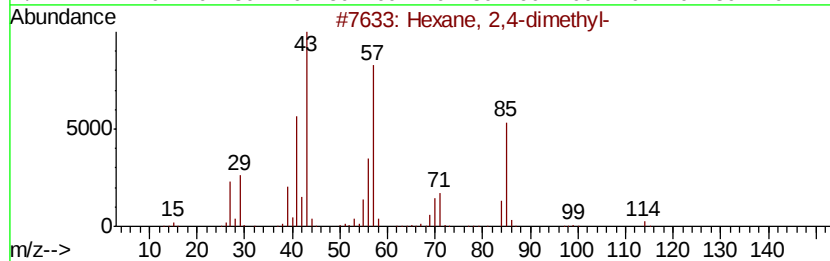
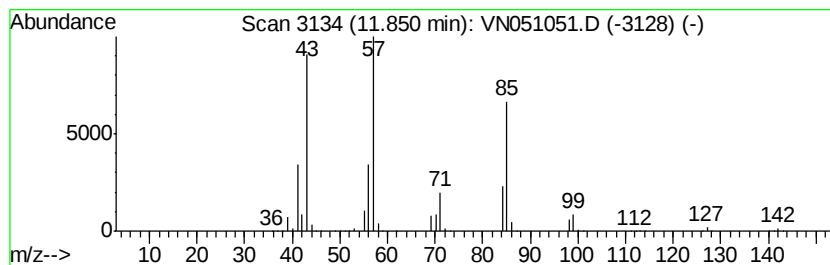
Instrument :
MSVOA_N
ClientSampleId :
EP1-MW-C(15-20)

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 6 Hexane, 2,4-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.85	118.28 ug/l	7245860	Chlorobenzene-d5	11.41
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Hexane, 2,4-dimethyl-	114 C8H18	000589-43-5	87
2	Heptane, 4,4-dimethyl-	128 C9H20	001068-19-5	50
3	Hexane, 1,1'-oxybis-	186 C12H26O	000112-58-3	50
4	Hexane, 2,2,3,3-tetramethyl-	142 C10H22	013475-81-5	50
5	Sulfurous acid, 2-ethylhexyl hex...	278 C14H30O3S	1000309-20-2	47



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_N\DATA\VN090718\
Data File : VN051051.D
Acq On : 7 Sep 2018 14:11
Operator : MD\SY
Sample : J4693-10
Misc : 5.91µL/5mL/100µL/5.00mL/MSVOA_N/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleID :
EP1-MW-C(15-20)

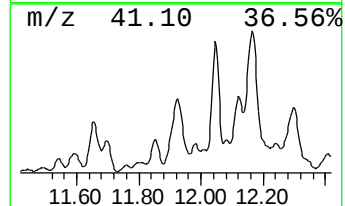
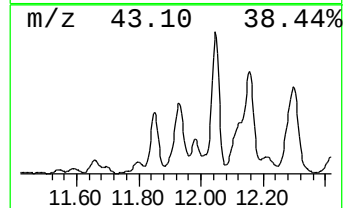
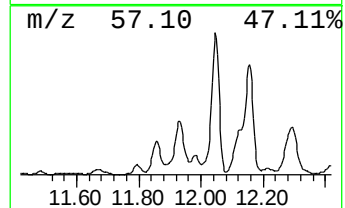
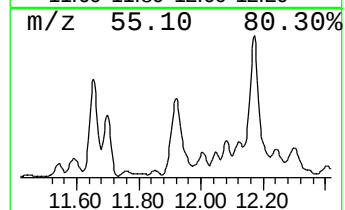
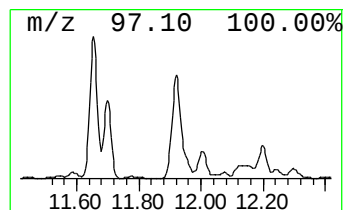
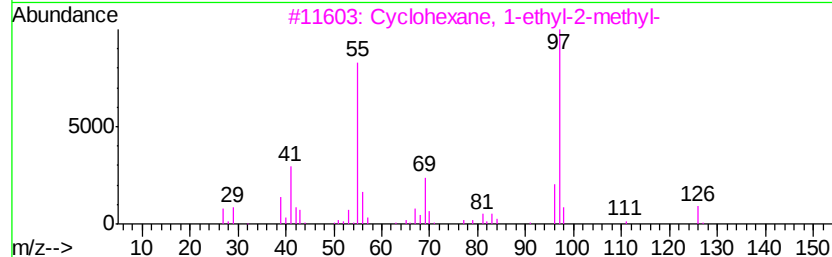
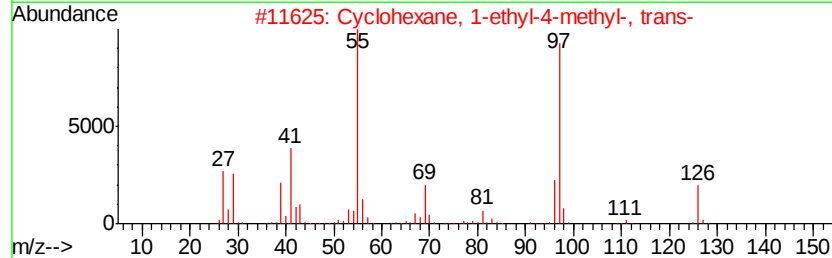
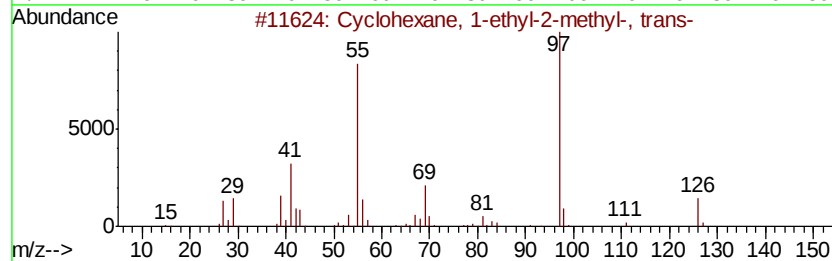
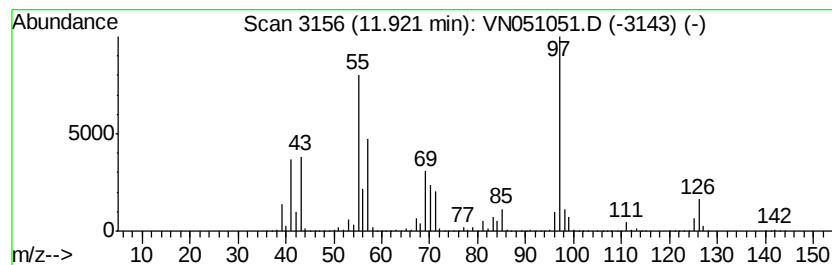
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Quant Title : SW846 8260

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

Peak Number 7 Cyclohexane, 1-ethyl-2-meth... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	633.28 ug/l	38794500	Chlorobenzene-d5	11.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-78-8	64
2		Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	006236-88-0	52
3		Cyclohexane, 1-ethyl-2-methyl-	126	C9H18	003728-54-9	52
4		3,5-Dimethyl-3-heptene	126	C9H18	059643-68-4	49
5		Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	47



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN090718\
Data File : VN051051.D
Acq On : 7 Sep 2018 14:11
Operator : MD\SY
Sample : J4693-10
Misc : 5.91µ/5mL/100µL/5.00mL/MSVOA_N/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
EP1-MW-C(15-20)

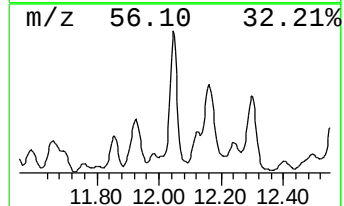
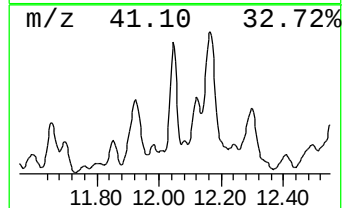
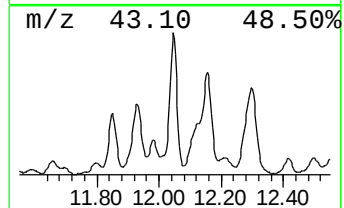
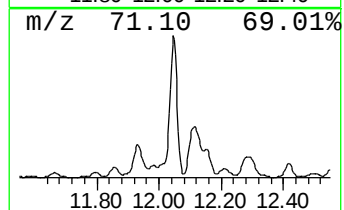
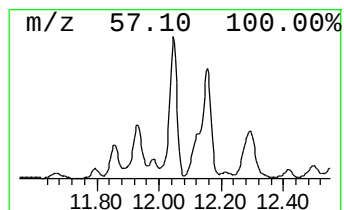
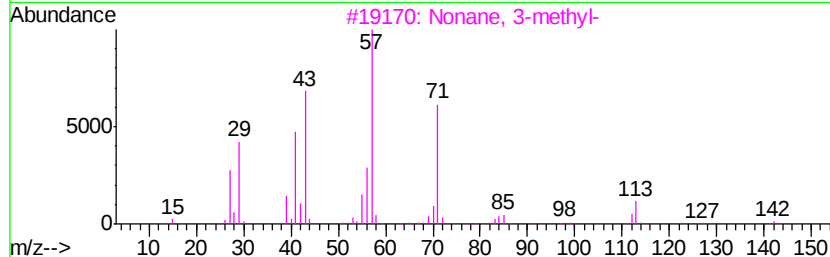
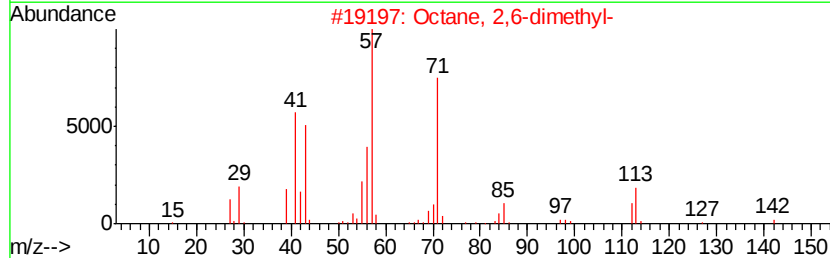
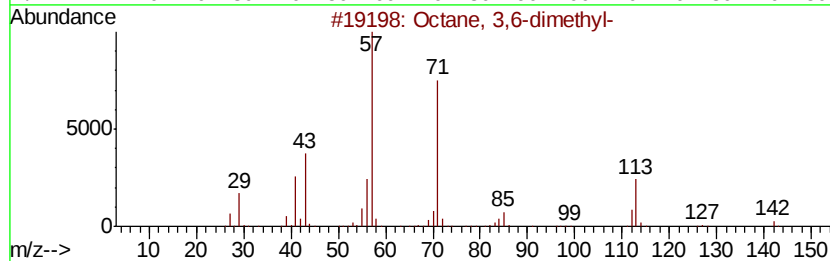
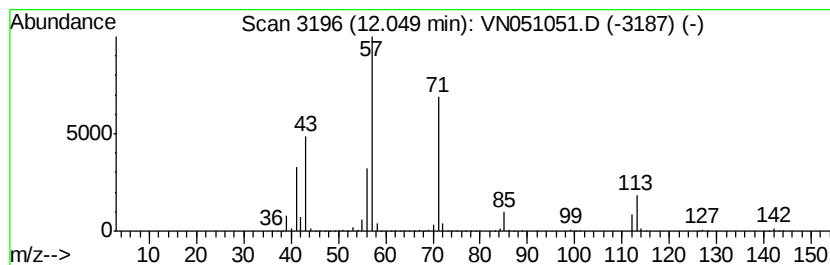
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.05	425.49 ug/l	26065300	Chlorobenzene-d5	11.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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		Heptane, 3-ethyl-5-methyl-	142	C10H22	052896-90-9	59
5		Nonane, 4-methyl-5-propyl-	184	C13H28	062185-55-1	59



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_N\DATA\VN090718\
Data File : VN051051.D
Acq On : 7 Sep 2018 14:11
Operator : MD\SY
Sample : J4693-10
Misc : 5.91µ/5mL/100µL/5.00mL/MSVOA_N/MEOH
ALS Vial : 12 Sample Multiplier: 1

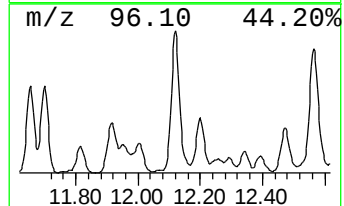
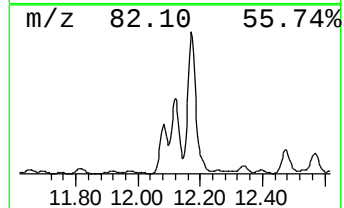
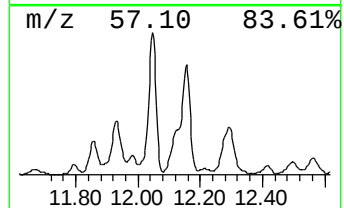
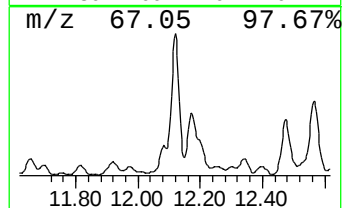
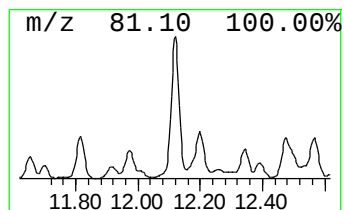
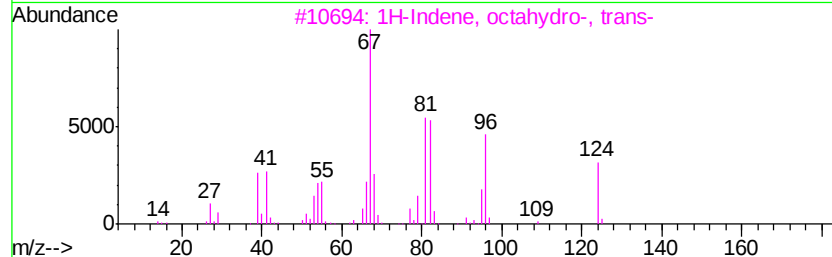
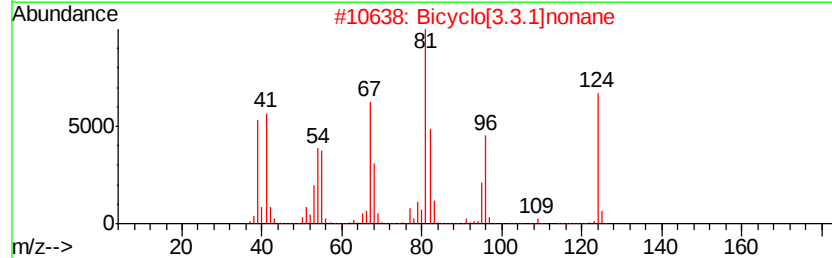
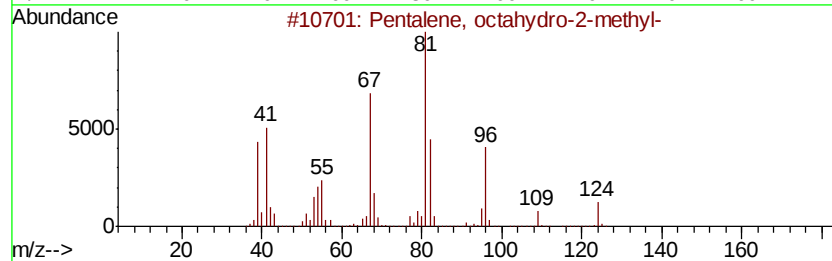
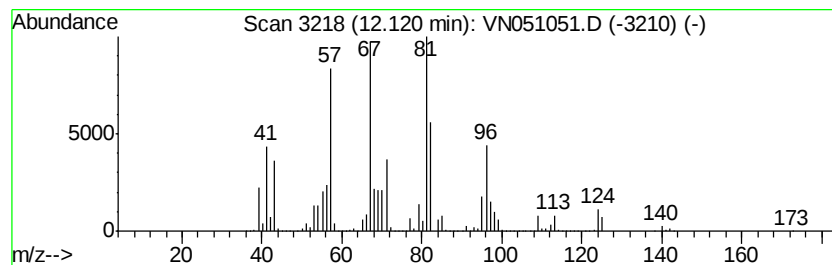
Instrument :
MSVOA_N
ClientSampleId :
EP1-MW-C(15-20)

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 9 Pentalene, octahydro-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.12	393.43 ug/l	24101600	Chlorobenzene-d5	11.41
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Pentalene, octahydro-2-methyl-	124 C9H16	003868-64-2 58
2		Bicyclo[3.3.1]nonane	124 C9H16	000280-65-9 58
3		1H-Indene, octahydro-, trans-	124 C9H16	003296-50-2 53
4		Cyclohexane, methylene-	96 C7H12	001192-37-6 50
5		3-Hexyne, 2-methyl-	96 C7H12	036566-80-0 43



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN090718\
Data File : VN051051.D
Acq On : 7 Sep 2018 14:11
Operator : MD\SY
Sample : J4693-10
Misc : 5.91µ/5mL/100µL/5.00mL/MSVOA_N/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
EP1-MW-C(15-20)

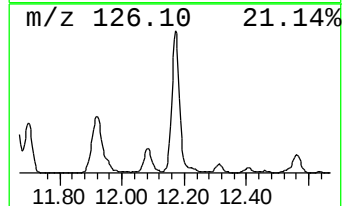
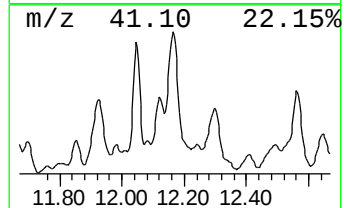
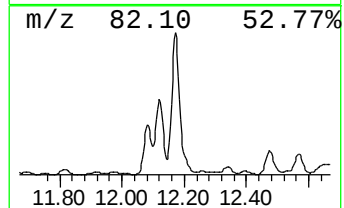
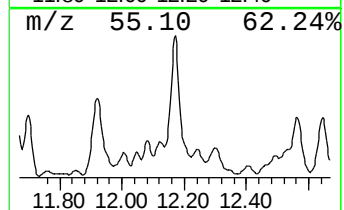
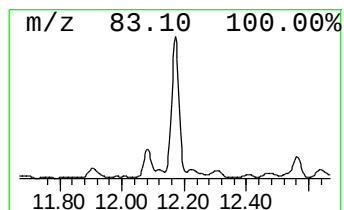
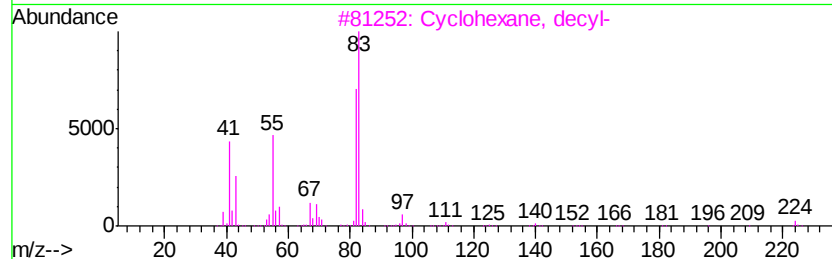
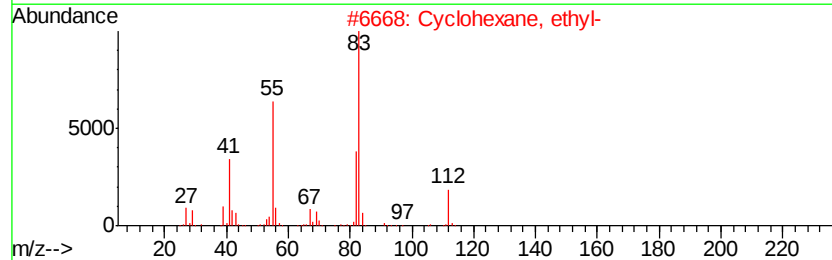
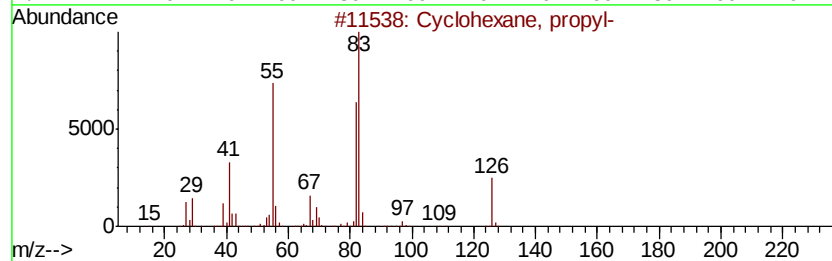
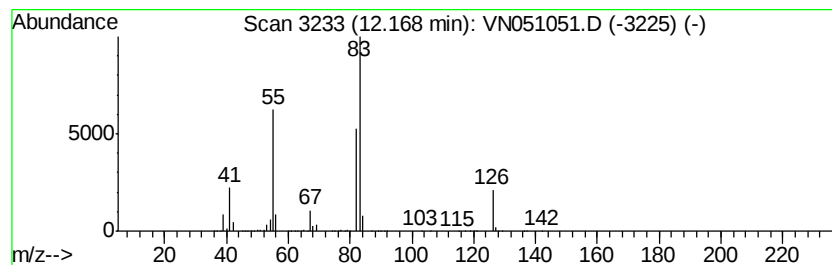
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N082118W.M
Quant Title : SW846 8260

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

Peak Number 10 Cyclohexane, propyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.17	752.72 ug/l	46111400	Chlorobenzene-d5	11.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, propyl-	126	C9H18	001678-92-8	87
2		Cyclohexane, ethyl-	112	C8H16	001678-91-7	64
3		Cyclohexane, decyl-	224	C16H32	001795-16-0	64
4		Cyclohexane, octyl-	196	C14H28	001795-15-9	64
5		Ethanone, 1-(1-methylcyclopentyl)-	126	C8H14O	013388-93-7	59



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN090718\
Data File : VN051051.D
Acq On : 7 Sep 2018 14:11
Operator : MD\SY
Sample : J4693-10
Misc : 5.91g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
EP1-MW-C(15-20)

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
Cyclohexane, 1,1,...	11.00	139.0	ug/l	8512620	3	11.41	3063000	50.0
Heptane, 2,3-dime...	11.12	117.3	ug/l	7185060	3	11.41	3063000	50.0
Cyclohexane, 1,2,...	11.21	153.7	ug/l	9415160	3	11.41	3063000	50.0
1-Ethyl-4-methylc...	11.65	361.3	ug/l	22130300	3	11.41	3063000	50.0
Cyclohexane, 1-et...	11.70	203.0	ug/l	12436400	3	11.41	3063000	50.0
Hexane, 2,4-dimet...	11.85	118.3	ug/l	7245860	3	11.41	3063000	50.0
Cyclohexane, 1-et...	11.92	633.3	ug/l	38794500	3	11.41	3063000	50.0
Octane, 3,6-dimet...	12.05	425.5	ug/l	26065300	3	11.41	3063000	50.0
Pentalene, octahy...	12.12	393.4	ug/l	24101600	3	11.41	3063000	50.0
Cyclohexane, propyl-	12.17	752.7	ug/l	46111400	3	11.41	3063000	50.0