

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN090718\
 Data File : VN051056.D
 Acq On : 7 Sep 2018 16:15
 Operator : MD\SY
 Sample : J4693-14 5X
 Misc : 6.44g/5mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 EP1-MW-D(7-10)

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	1789	1810	1821	rBV	470396	1185022	1.34%	0.136%
2	7.667	1821	1833	1850	rVB	726142	1688921	1.92%	0.194%
3	8.027	1925	1945	1972	rBV	462134	1067507	1.21%	0.123%
4	8.586	2102	2119	2142	rBV	1031531	2147076	2.44%	0.247%
5	10.091	2573	2587	2612	rVB	2292995	4638161	5.26%	0.533%
6	10.432	2685	2693	2709	rVB	1065774	2026909	2.30%	0.233%
7	10.532	2710	2724	2733	rBV2	633758	1368451	1.55%	0.157%
8	10.628	2745	2754	2763	rVB	764192	1225569	1.39%	0.141%
9	10.718	2771	2782	2795	rVB	3674334	6130434	6.95%	0.704%
10	10.821	2797	2814	2827	rBV	1994780	4433486	5.03%	0.509%
11	10.889	2827	2835	2841	rBV2	836407	1411152	1.60%	0.162%
12	11.008	2858	2872	2883	rBV	8968652	17199033	19.51%	1.976%
13	11.059	2883	2888	2896	rVV	1255710	1919002	2.18%	0.220%
14	11.123	2896	2908	2916	rVV5	4730723	8990733	10.20%	1.033%
15	11.207	2916	2934	2951	rVB6	5772855	17521578	19.87%	2.013%
16	11.291	2951	2960	2969	rBV	1529560	2568691	2.91%	0.295%
17	11.406	2987	2996	3003	rBV	1442412	2493846	2.83%	0.287%
18	11.493	3016	3023	3030	rBV3	648526	1123911	1.27%	0.129%
19	11.545	3030	3039	3045	rVV	3174919	4948311	5.61%	0.569%
20	11.596	3045	3055	3064	rVV7	5362750	11913985	13.51%	1.369%
21	11.657	3064	3074	3081	rVV2	11633616	22245203	25.23%	2.556%
22	11.699	3082	3087	3097	rVB2	8436311	13177219	14.95%	1.514%
23	11.760	3097	3106	3113	rBV3	1936804	3572153	4.05%	0.410%
24	11.853	3128	3135	3143	rVB4	2988807	4478038	5.08%	0.514%
25	11.924	3143	3157	3170	rBV6	14074656	35245992	39.98%	4.049%
26	12.046	3188	3195	3203	rBV	18140835	24910418	28.26%	2.862%
27	12.123	3211	3219	3223	rBV3	9586565	14803810	16.79%	1.701%
28	12.165	3224	3232	3249	rVB4	20792928	42431055	48.13%	4.875%
29	12.406	3296	3307	3316	rBV6	4595556	9373961	10.63%	1.077%
30	12.490	3317	3333	3340	rBV7	5437038	15973007	18.12%	1.835%
31	12.564	3348	3356	3372	rVB3	21734577	48455105	54.96%	5.567%
32	12.647	3372	3382	3391	rBV6	7890471	16695819	18.94%	1.918%
33	12.731	3393	3408	3417	rVV5	23997056	67167164	76.19%	7.717%
34	12.782	3418	3424	3434	rVB3	14052825	22405528	25.41%	2.574%

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35	12.869	3444	3451	3458	rBV4	6782820	9606090	10.90%	1.104%
36	12.911	3459	3464	3466	rBV2	2825340	2986533	3.39%	0.343%
37	12.966	3473	3481	3494	rVB3	22647983	39634017	44.96%	4.553%
38	13.043	3495	3505	3515	rBV2	52108442	88159313	100.00%	10.128%
39	13.172	3532	3545	3553	rBV6	10210006	21412647	24.29%	2.460%
40	13.242	3554	3567	3574	rBV	17575426	32199854	36.52%	3.699%
41	13.596	3668	3677	3689	rBV2	12786759	30135944	34.18%	3.462%
42	13.663	3690	3698	3708	rVV5	18563069	35045550	39.75%	4.026%
43	13.712	3710	3713	3721	rVB2	3547430	4304766	4.88%	0.495%
44	13.802	3735	3741	3746	rBV2	9735084	14405157	16.34%	1.655%
45	13.834	3747	3751	3760	rVV	14690685	20452701	23.20%	2.350%
46	13.889	3761	3768	3778	rVB	19259024	30300866	34.37%	3.481%
47	13.995	3792	3801	3812	rVB5	9748301	18264646	20.72%	2.098%
48	14.072	3817	3825	3833	rVV5	3648316	6328884	7.18%	0.727%
49	14.178	3849	3858	3863	rBV5	6286205	11419896	12.95%	1.312%
50	14.249	3874	3880	3888	rVB	11831791	16801292	19.06%	1.930%
51	14.294	3888	3894	3900	rBV3	2979767	3535486	4.01%	0.406%
52	14.332	3901	3906	3912	rVV2	2509639	2894276	3.28%	0.333%
53	14.480	3944	3952	3959	rBV3	2435580	4984710	5.65%	0.573%
54	14.525	3960	3966	3974	rVV	4244703	6236340	7.07%	0.716%
55	14.583	3974	3984	3997	rVV2	12587508	23756502	26.95%	2.729%
56	14.647	3997	4004	4015	rVB	2536918	4237593	4.81%	0.487%
57	14.853	4061	4068	4073	rBV4	1584294	2335402	2.65%	0.268%
58	14.956	4092	4100	4112	rVB3	1962465	4034182	4.58%	0.463%

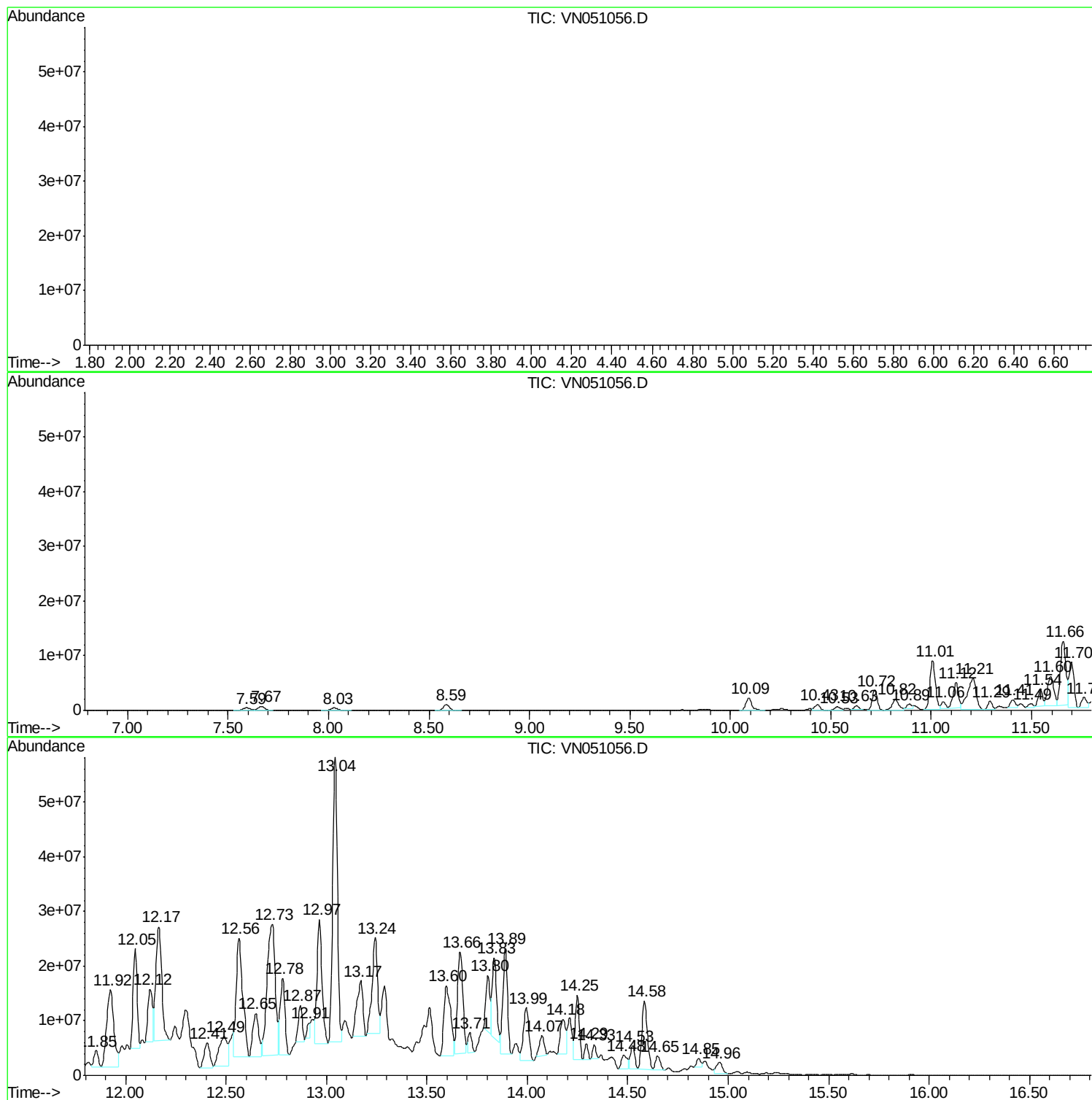
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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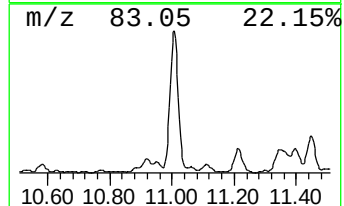
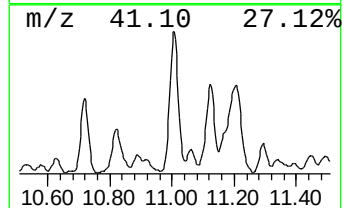
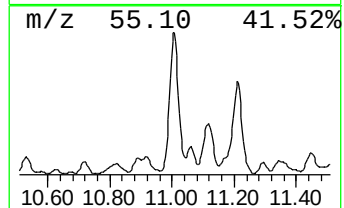
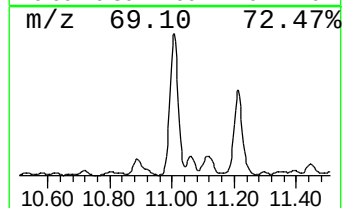
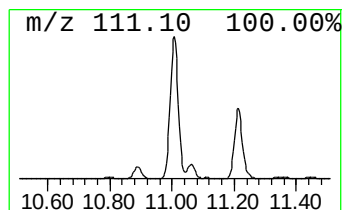
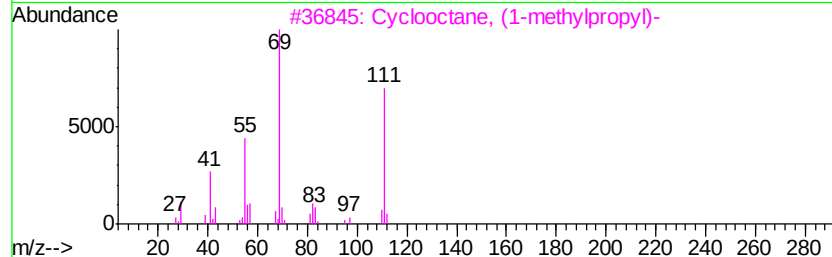
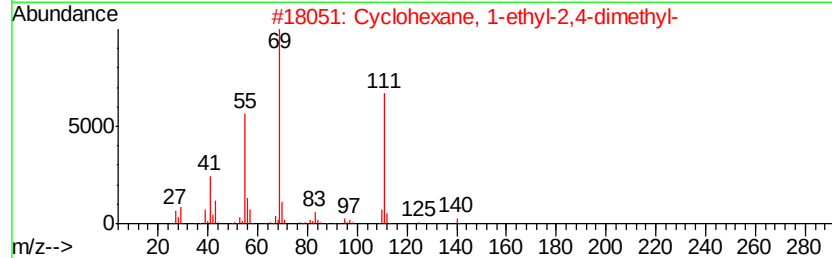
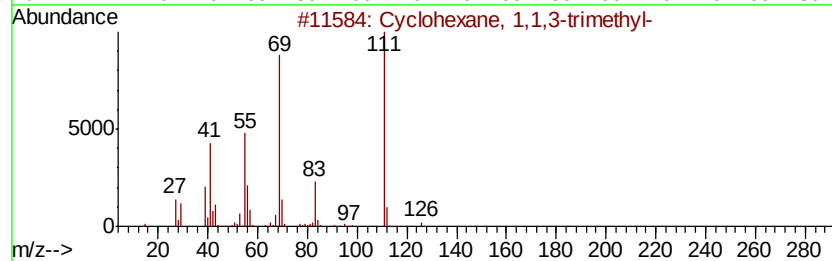
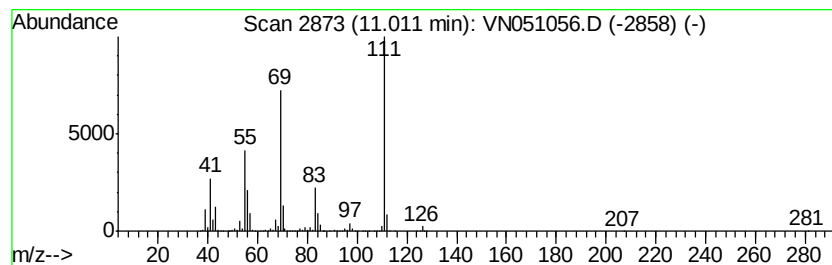
Instrument :
MSVOA_N
ClientSampleId :
EP1-MW-D(7-10)

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 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.01	344.83 ug/l	17199000	Chlorobenzene-d5	11.41
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Cyclohexane, 1,1,3-trimethyl-	126 C9H18	003073-66-3 95
2		Cyclohexane, 1-ethyl-2,4-dimethyl-	140 C10H20	061142-69-6 72
3		Cyclooctane, (1-methylpropyl)-	168 C12H24	016538-89-9 59
4		Cyclohexane, 1,3,5-trimethyl-, (...)	126 C9H18	001795-26-2 50
5		4-Amino-6-hydroxypyrimidine	111 C4H5N3O	001193-22-2 50



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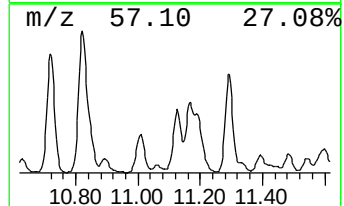
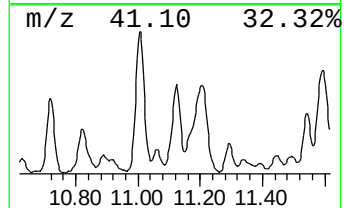
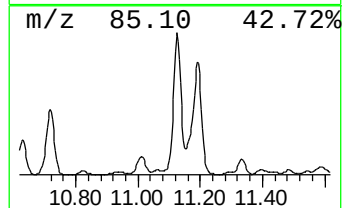
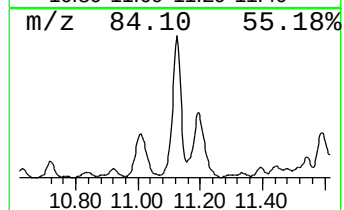
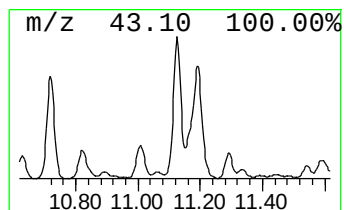
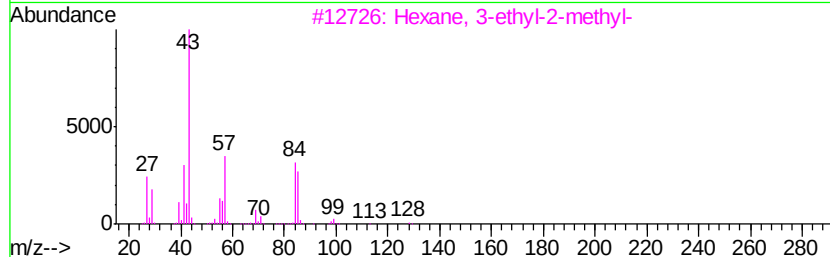
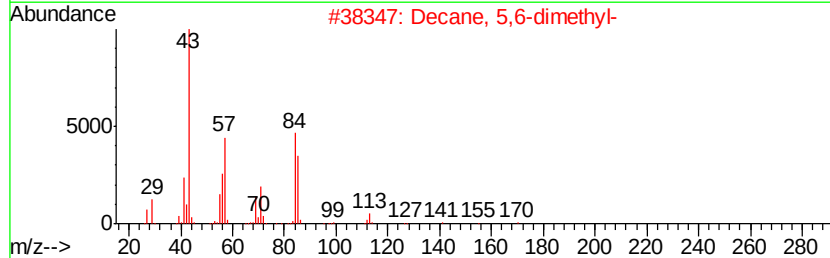
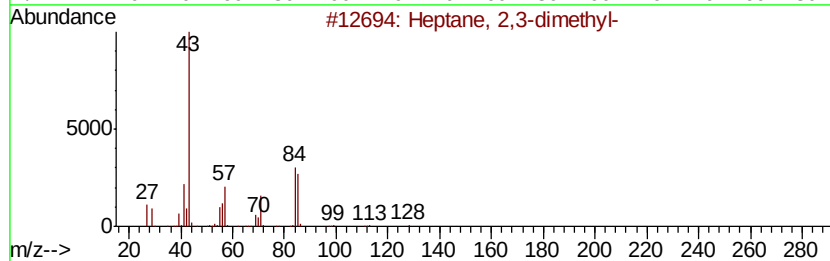
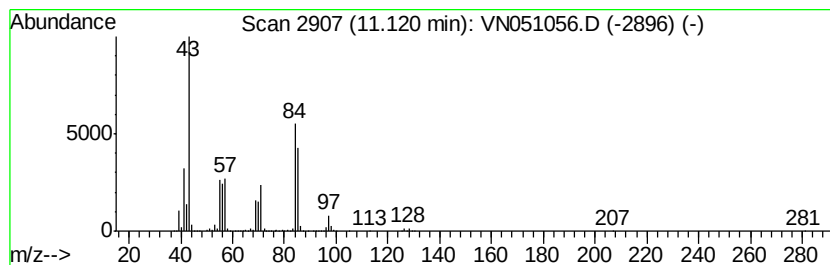
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.12	180.26 ug/l	8990730	Chlorobenzene-d5	11.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptane, 2,3-dimethyl-	128	C9H20	003074-71-3	87
2		Decane, 5,6-dimethyl-	170	C12H26	001636-43-7	59
3		Hexane, 3-ethyl-2-methyl-	128	C9H20	016789-46-1	58
4		Hexane, 2,3,5-trimethyl-	128	C9H20	001069-53-0	58
5		Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	53



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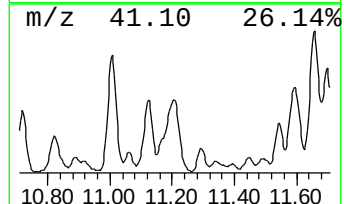
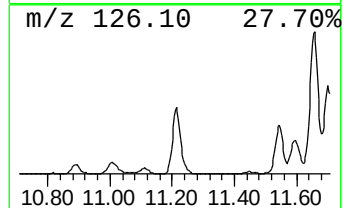
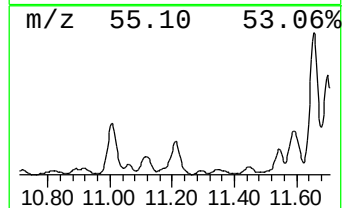
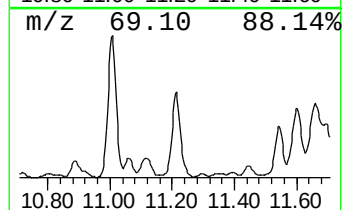
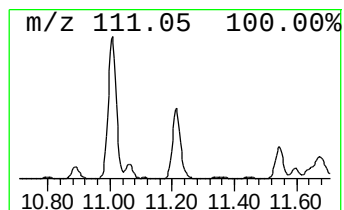
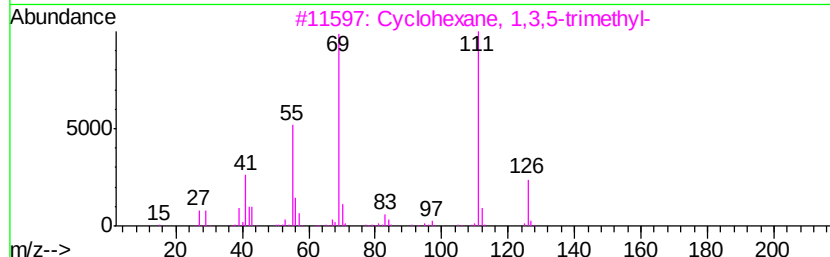
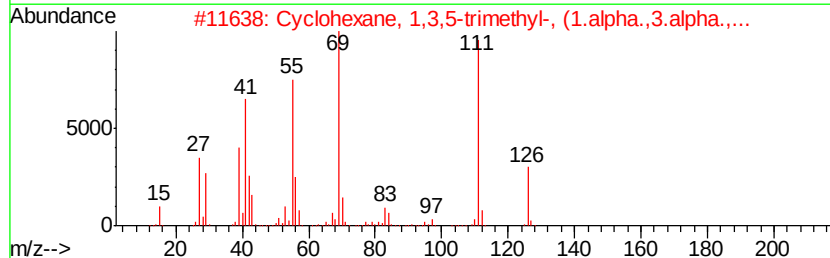
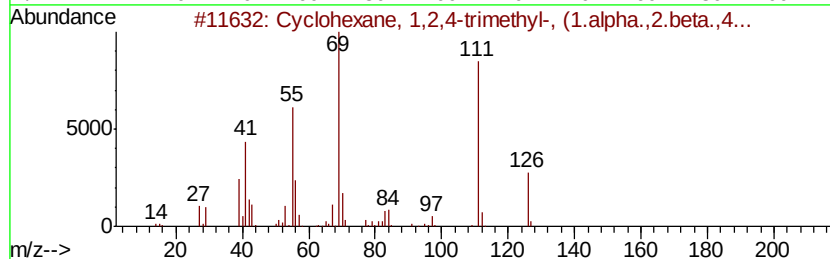
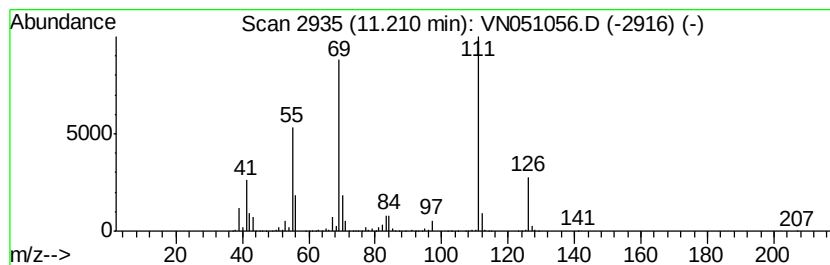
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.21	351.30 ug/l	17521600	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	001795-26-2	87
3		Cyclohexane, 1,3,5-trimethyl-	126	C9H18	001839-63-0	74
4		Cyclohexane, 1,3,5-trimethyl-, (...	126	C9H18	001795-27-3	74
5		Cyclohexane, 1,2,4-trimethyl-	126	C9H18	002234-75-5	70



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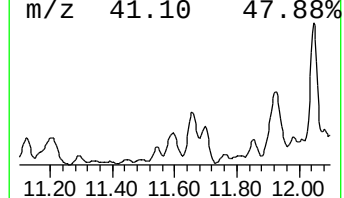
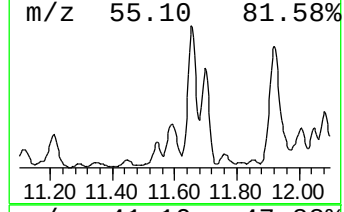
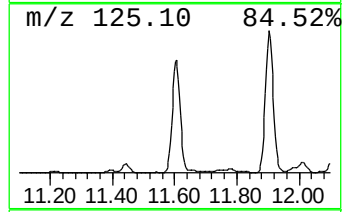
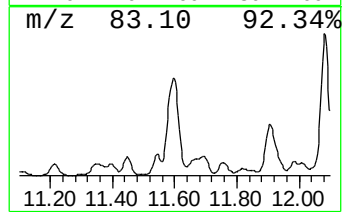
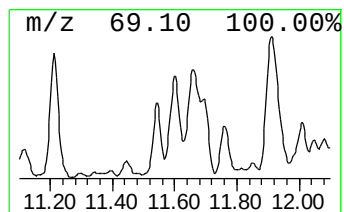
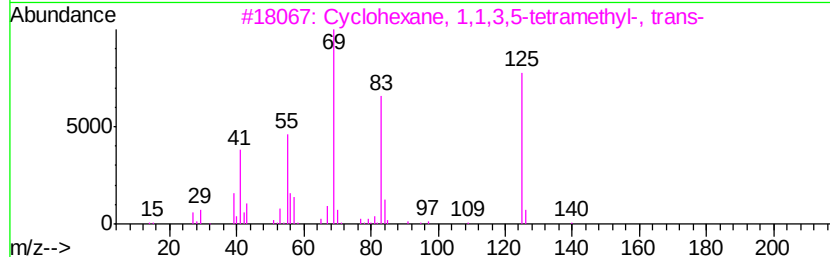
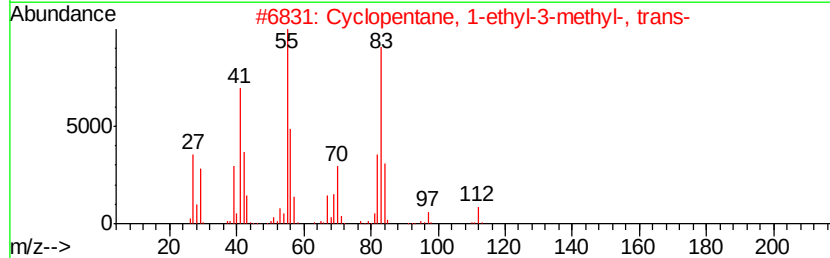
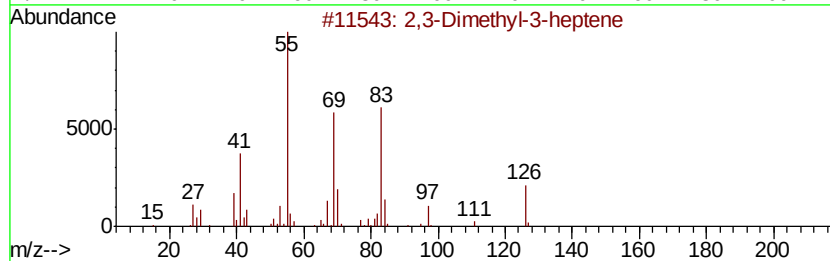
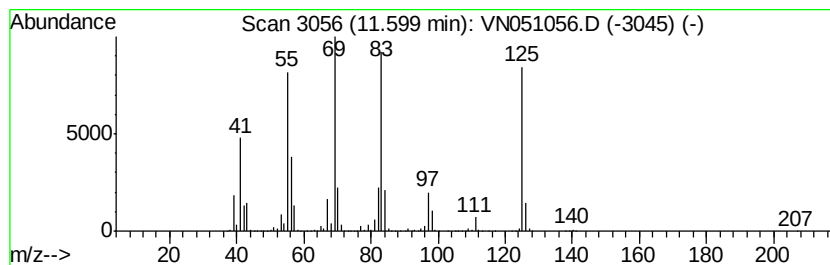
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TIC Integration Parameters: LSCINT.P

Peak Number 4 2,3-Dimethyl-3-heptene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.60	238.87 ug/l	11914000	Chlorobenzene-d5	11.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2,3-Dimethyl-3-heptene	126	C9H18	1000113-49-3	60
2		Cyclopentane, 1-ethyl-3-methyl-, ...	112	C8H16	002613-65-2	50
3		Cyclohexane, 1,1,3,5-tetramethyl...	140	C10H20	050876-31-8	49
4		Cyclopentane, 1-ethyl-3-methyl-	112	C8H16	003726-47-4	38
5		Cyclopentane, 1-methyl-2-propyl-	126	C9H18	003728-57-2	30



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Misc : 6.44g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

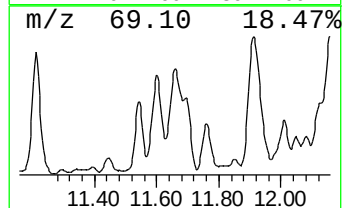
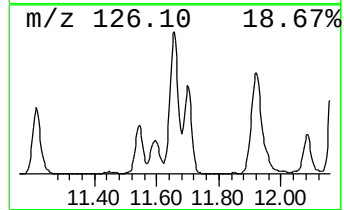
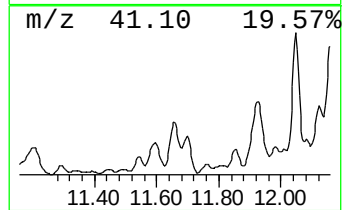
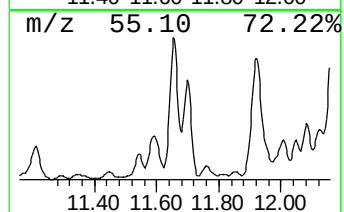
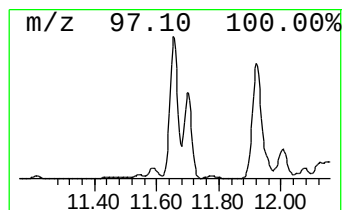
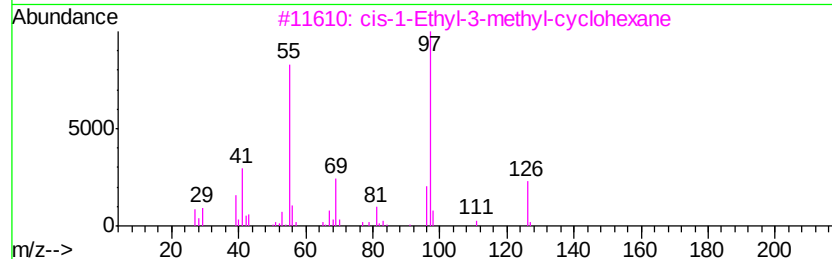
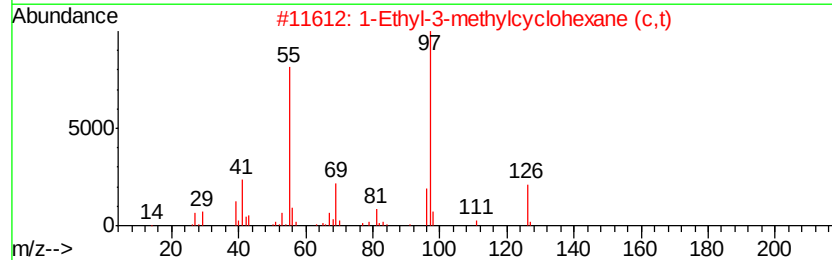
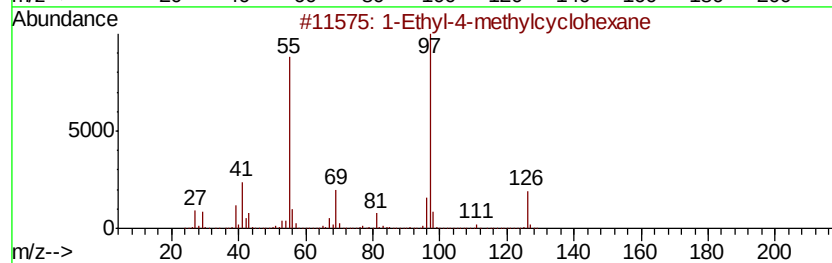
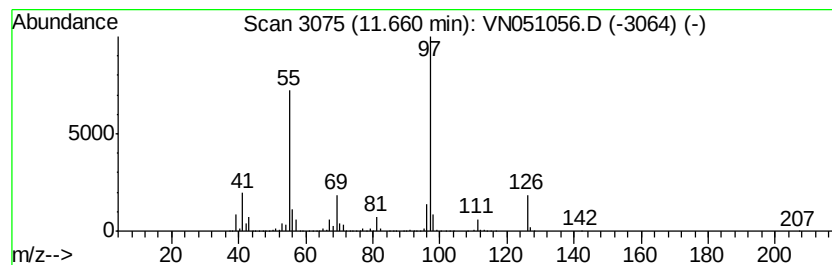
Instrument :
MSVOA_N
ClientSampleId :
EP1-MW-D(7-10)

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 5 1-Ethyl-4-methylcyclohexane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.66	446.00 ug/l	22245200	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		1-Ethyl-3-methylcyclohexane (c,t)	126 C9H18	003728-55-0 91
3		cis-1-Ethyl-3-methyl-cyclohexane	126 C9H18	019489-10-2 91
4		3,5-Dimethyl-3-heptene	126 C9H18	059643-68-4 87
5		Cyclohexane, 1-ethyl-4-methyl-, ...	126 C9H18	004926-78-7 87



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_N\DATA\VN090718\
Data File : VN051056.D
Acq On : 7 Sep 2018 16:15
Operator : MD\SY
Sample : J4693-14 5X
Misc : 6.44g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

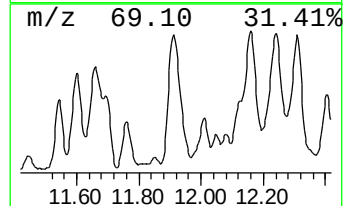
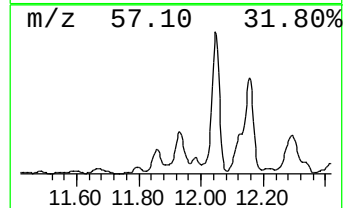
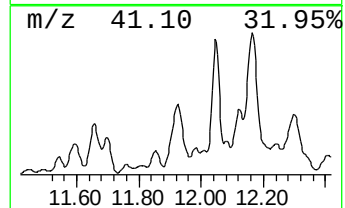
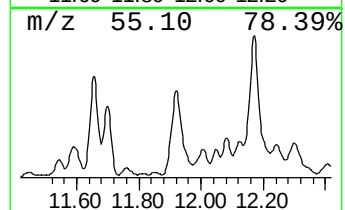
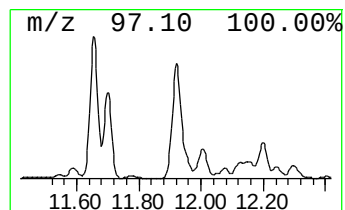
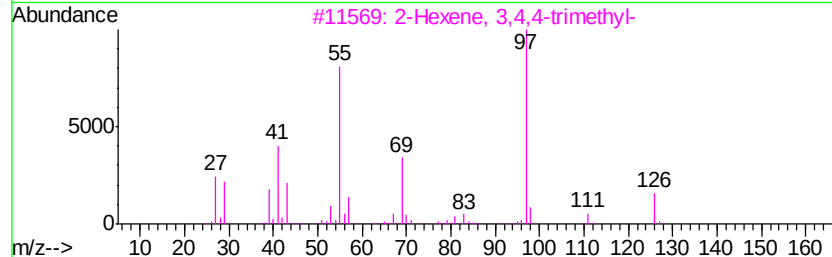
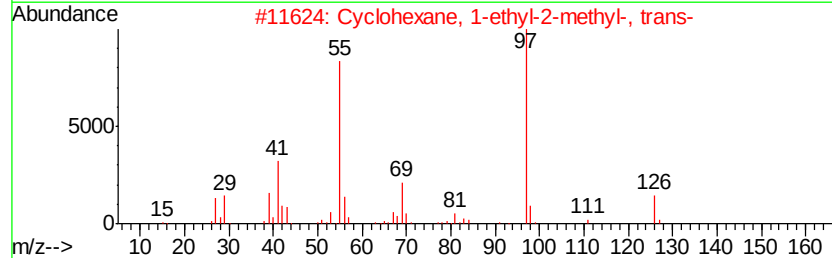
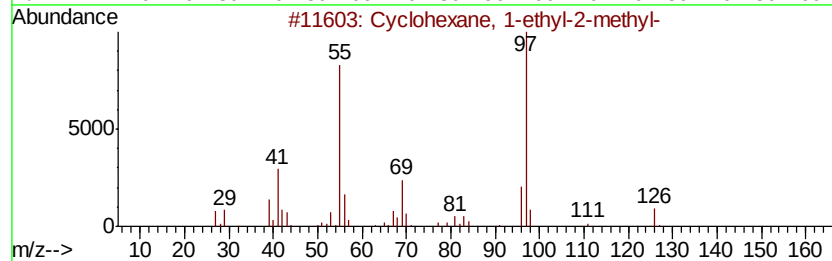
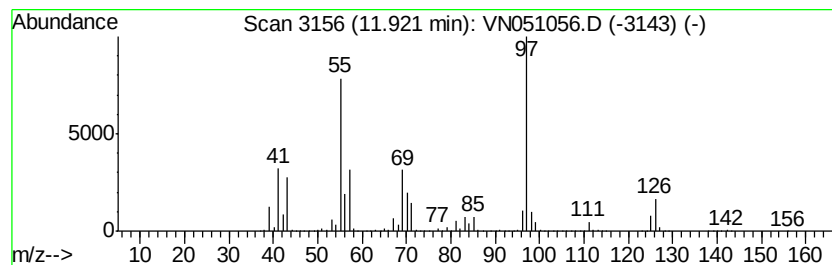
Instrument :
MSVOA_N
ClientSampleId :
EP1-MW-D(7-10)

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 Cyclohexane, 1-ethyl-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.		
11.92	706.66 ug/l	35246000	Chlorobenzene-d5	11.41		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclohexane, 1-ethyl-2-methyl-	126	C9H18	003728-54-9	72
2		Cyclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-78-8	64
3		2-Hexene, 3,4,4-trimethyl-	126	C9H18	053941-19-8	58
4		Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	006236-88-0	58
5		Sulfurous acid, cyclohexylmethyl...	430	C25H50O3S	1000309-22-6	53



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_N\DATA\VN090718\
Data File : VN051056.D
Acq On : 7 Sep 2018 16:15
Operator : MD\SY
Sample : J4693-14 5X
Misc : 6.44g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
EP1-MW-D(7-10)

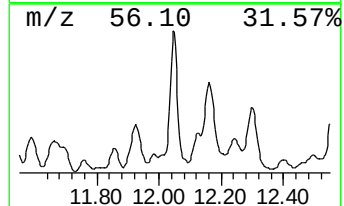
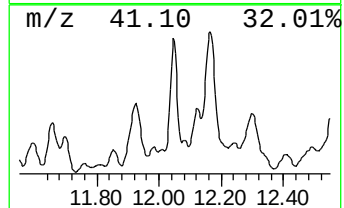
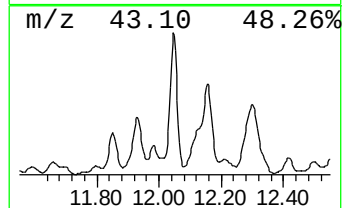
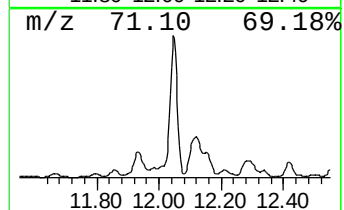
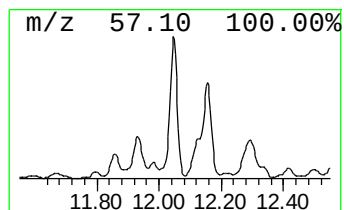
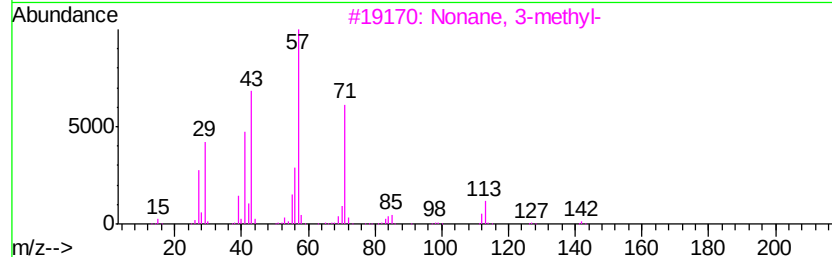
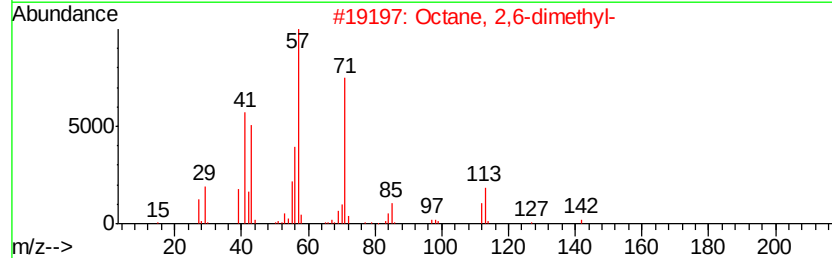
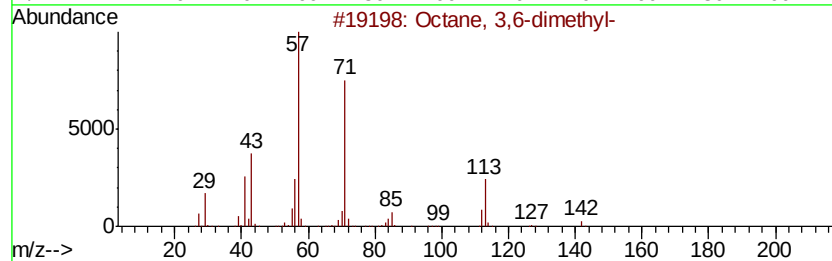
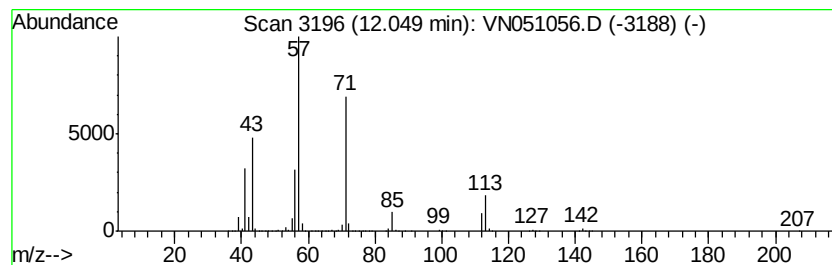
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Quant Title : SW846 8260

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	499.44 ug/l	24910400	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		Undecane, 6,6-dimethyl-	184	C13H28	017312-76-4	64
5		Nonane, 4-methyl-5-propyl-	184	C13H28	062185-55-1	59



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN090718\
Data File : VN051056.D
Acq On : 7 Sep 2018 16:15
Operator : MD\SY
Sample : J4693-14 5X
Misc : 6.44g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

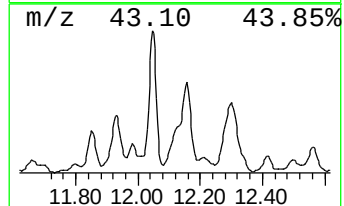
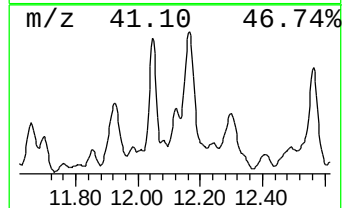
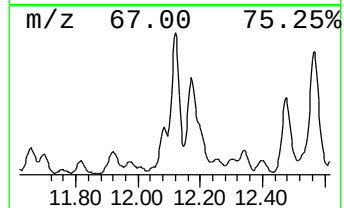
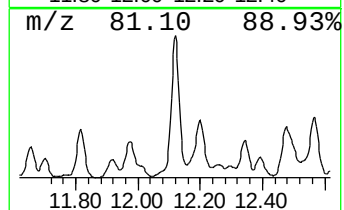
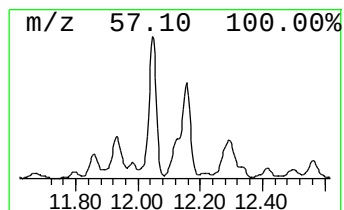
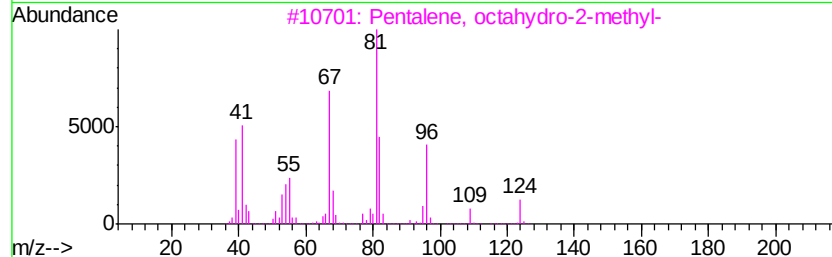
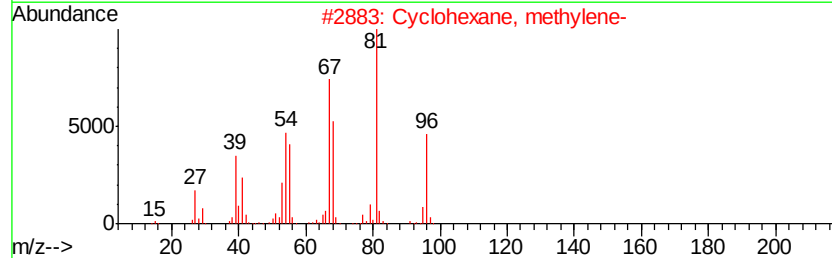
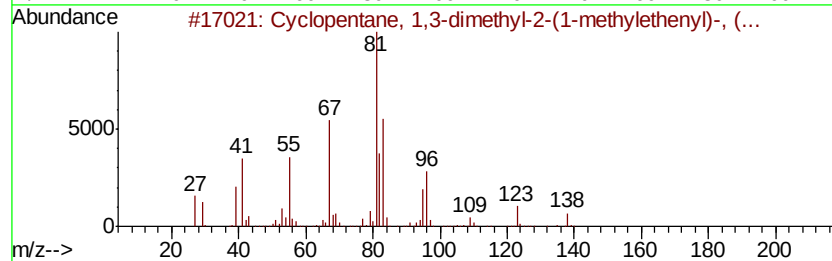
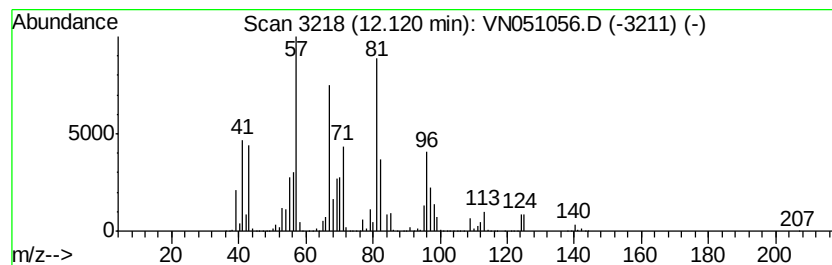
Instrument :
MSVOA_N
ClientSampleId :
EP1-MW-D(7-10)

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 9 Cyclopentane, 1,3-dimethyl-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.		
12.12	296.81 ug/l	14803800	Chlorobenzene-d5	11.41		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopentane, 1,3-dimethyl-2-(1-...	138	C10H18	061142-31-2	53
2		Cyclohexane, methylene-	96	C7H12	001192-37-6	52
3		Pentalene, octahydro-2-methyl-	124	C9H16	003868-64-2	47
4		Cyclohexene, 1-methyl-	96	C7H12	000591-49-1	43
5		1H-Indene, octahydro-, trans-	124	C9H16	003296-50-2	30



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_N\DATA\VN090718\
Data File : VN051056.D
Acq On : 7 Sep 2018 16:15
Operator : MD\SY
Sample : J4693-14 5X
Misc : 6.44g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

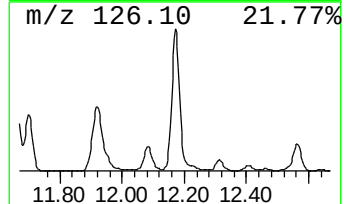
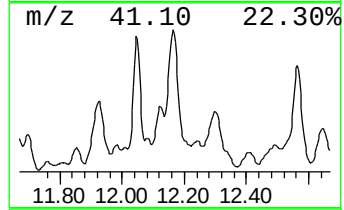
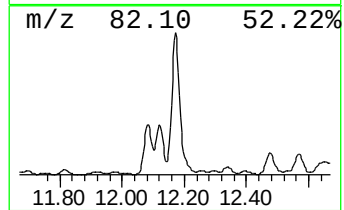
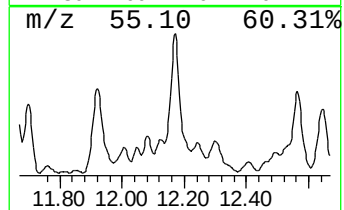
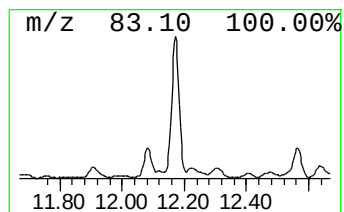
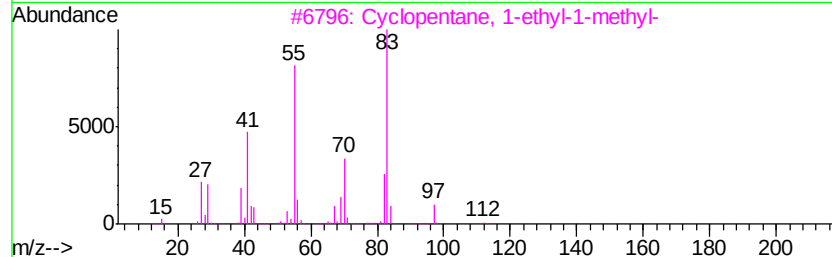
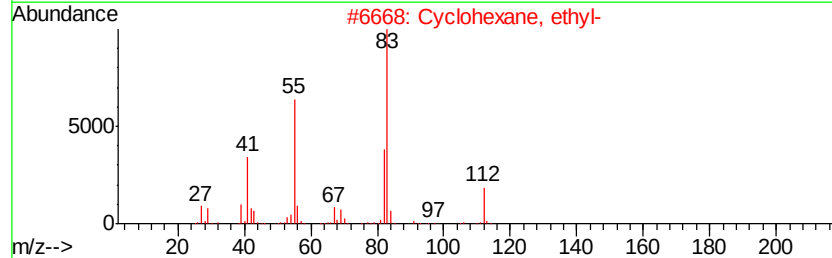
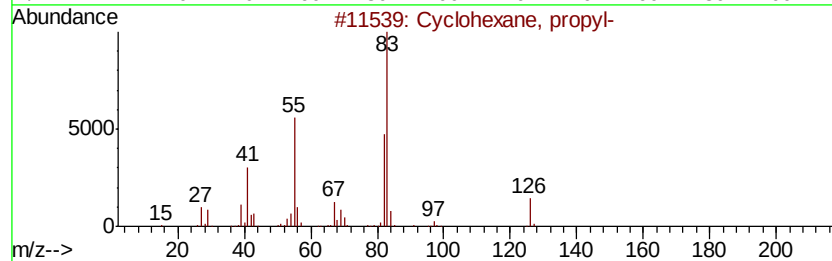
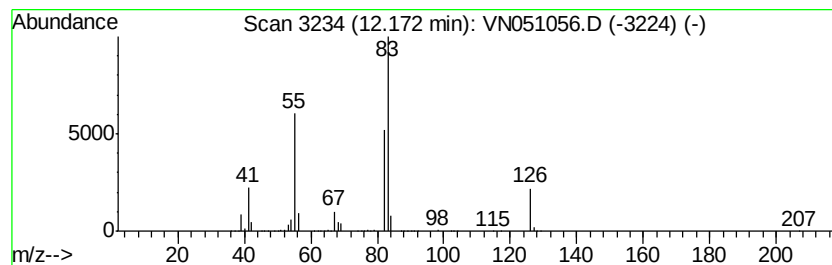
Instrument :
MSVOA_N
ClientSampleId :
EP1-MW-D(7-10)

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	850.72 ug/l	42431100	Chlorobenzene-d5	11.41		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclohexane, propyl-	126	C9H18	001678-92-8	86
2		Cyclohexane, ethyl-	112	C8H16	001678-91-7	59
3		Cyclopentane, 1-ethyl-1-methyl-	112	C8H16	016747-50-5	59
4		Oxalic acid, cyclohexyl dodecyl ...	340	C20H36O4	1000309-31-4	53
5		Ethanone, 1-(1-methylcyclopentyl)-	126	C8H14O	013388-93-7	53



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN090718\
Data File : VN051056.D
Acq On : 7 Sep 2018 16:15
Operator : MD\SY
Sample : J4693-14 5X
Misc : 6.44g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
EP1-MW-D(7-10)

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,...	11.01	344.8	ug/l	17199000	3	11.41	2493850	50.0
Heptane, 2,3-dime...	11.12	180.3	ug/l	8990730	3	11.41	2493850	50.0
Cyclohexane, 1,2,...	11.21	351.3	ug/l	17521600	3	11.41	2493850	50.0
2,3-Dimethyl-3-he...	11.60	238.9	ug/l	11914000	3	11.41	2493850	50.0
1-Ethyl-4-methylc...	11.66	446.0	ug/l	22245200	3	11.41	2493850	50.0
Cyclohexane, 1-et...	11.92	706.7	ug/l	35246000	3	11.41	2493850	50.0
Octane, 3,6-dimet...	12.05	499.4	ug/l	24910400	3	11.41	2493850	50.0
Cyclopentane, 1,3...	12.12	296.8	ug/l	14803800	3	11.41	2493850	50.0
Cyclohexane, propyl-	12.17	850.7	ug/l	42431100	3	11.41	2493850	50.0