

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN100618\
 Data File : VN051716.D
 Acq On : 6 Oct 2018 3:45
 Operator : MD\SY
 Sample : J5165-05 40X
 Misc : 6.24g/5.00mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 46 Sample Multiplier: 28

Instrument :
 MSVOA_N
 ClientSampleId :
 EP1-MW-D-092718(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\82N100418W.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	2.445	198	209	223	rBV5	41363	103976	1.63%	0.118%
2	7.593	1791	1810	1821	rBV	516452	1276461	19.97%	1.448%
3	7.667	1822	1833	1864	rVB	795810	1906557	29.83%	2.163%
4	8.030	1926	1946	1973	rBV	488388	1154910	18.07%	1.310%
5	8.587	2102	2119	2149	rBV	1077775	2251401	35.22%	2.554%
6	10.091	2571	2587	2616	rBV	1969681	3698166	57.86%	4.195%
7	10.435	2685	2694	2706	rVB2	95296	179448	2.81%	0.204%
8	10.532	2710	2724	2733	rBV4	49632	110978	1.74%	0.126%
9	10.628	2746	2754	2763	rVB4	57050	91576	1.43%	0.104%
10	10.718	2772	2782	2796	rVB	295882	497320	7.78%	0.564%
11	10.821	2798	2814	2827	rBV	151862	350638	5.49%	0.398%
12	10.889	2828	2835	2841	rBV3	54898	93949	1.47%	0.107%
13	11.008	2857	2872	2882	rBV	772813	1505289	23.55%	1.707%
14	11.059	2883	2888	2896	rVV2	116565	195919	3.07%	0.222%
15	11.123	2896	2908	2916	rVV4	368112	729802	11.42%	0.828%
16	11.168	2917	2922	2924	rVV4	127943	155795	2.44%	0.177%
17	11.210	2926	2935	2951	rVB2	411282	893683	13.98%	1.014%
18	11.291	2951	2960	2968	rBV2	105324	172879	2.70%	0.196%
19	11.410	2984	2997	3016	rBV	1469502	2746902	42.97%	3.116%
20	11.541	3029	3038	3045	rBV	256440	411250	6.43%	0.466%
21	11.599	3045	3056	3064	rVV6	360457	771618	12.07%	0.875%
22	11.654	3064	3073	3081	rVV	776467	1511791	23.65%	1.715%
23	11.699	3082	3087	3097	rVB2	567508	885172	13.85%	1.004%
24	11.760	3097	3106	3113	rBV4	164482	305665	4.78%	0.347%
25	11.853	3128	3135	3143	rVB4	280057	428742	6.71%	0.486%
26	11.924	3143	3157	3169	rBV6	1211137	2944437	46.07%	3.340%
27	12.046	3187	3195	3203	rVB	1894130	2609557	40.83%	2.960%
28	12.120	3211	3218	3222	rBV3	609643	912213	14.27%	1.035%
29	12.152	3224	3228	3237	rVB	1127761	1582552	24.76%	1.795%
30	12.201	3238	3243	3249	rBV5	233747	362476	5.67%	0.411%
31	12.403	3295	3306	3317	rBV3	1685183	2992427	46.82%	3.394%
32	12.490	3317	3333	3340	rBV8	504936	1454700	22.76%	1.650%
33	12.561	3348	3355	3369	rVB4	2038647	3885817	60.79%	4.408%
34	12.647	3370	3382	3391	rBV6	837033	1999966	31.29%	2.269%

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35	12.728	3393	3407	3416	rVV5	2324559	6291443	98.43%	7.136%
36	12.779	3419	3423	3433	rVB3	1317696	1943433	30.40%	2.204%
37	12.869	3444	3451	3458	rBV4	773405	1130751	17.69%	1.283%
38	12.963	3472	3480	3493	rVB2	3879475	6391872	100.00%	7.250%
39	13.088	3514	3519	3529	rVB4	525261	788542	12.34%	0.894%
40	13.168	3531	3544	3552	rBV6	1200909	2861859	44.77%	3.246%
41	13.239	3554	3566	3574	rBV2	1887004	3408446	53.32%	3.866%
42	13.345	3590	3599	3611	rVB	1623229	2948485	46.13%	3.345%
43	13.596	3668	3677	3688	rBV2	1202353	2595917	40.61%	2.945%
44	13.663	3689	3698	3708	rVV5	2083954	3963163	62.00%	4.495%
45	13.802	3736	3741	3747	rVB	855220	946664	14.81%	1.074%
46	13.889	3761	3768	3777	rVB	2614497	3987585	62.39%	4.523%
47	13.991	3792	3800	3811	rVB5	704018	1369335	21.42%	1.553%
48	14.178	3849	3858	3863	rBV5	887516	1576784	24.67%	1.789%
49	14.249	3874	3880	3888	rVB	1682186	2423293	37.91%	2.749%
50	14.294	3888	3894	3900	rBV3	343404	404000	6.32%	0.458%
51	14.332	3900	3906	3912	rBV3	384202	473532	7.41%	0.537%
52	14.480	3945	3952	3959	rBV5	178926	355494	5.56%	0.403%
53	14.525	3959	3966	3974	rVV	544522	817693	12.79%	0.928%
54	14.583	3975	3984	3996	rVV5	478498	1077643	16.86%	1.222%
55	14.647	3997	4004	4015	rVB3	341785	607180	9.50%	0.689%
56	14.853	4063	4068	4072	rBV5	96246	105782	1.65%	0.120%
57	14.956	4092	4100	4112	rVB2	248589	516032	8.07%	0.585%

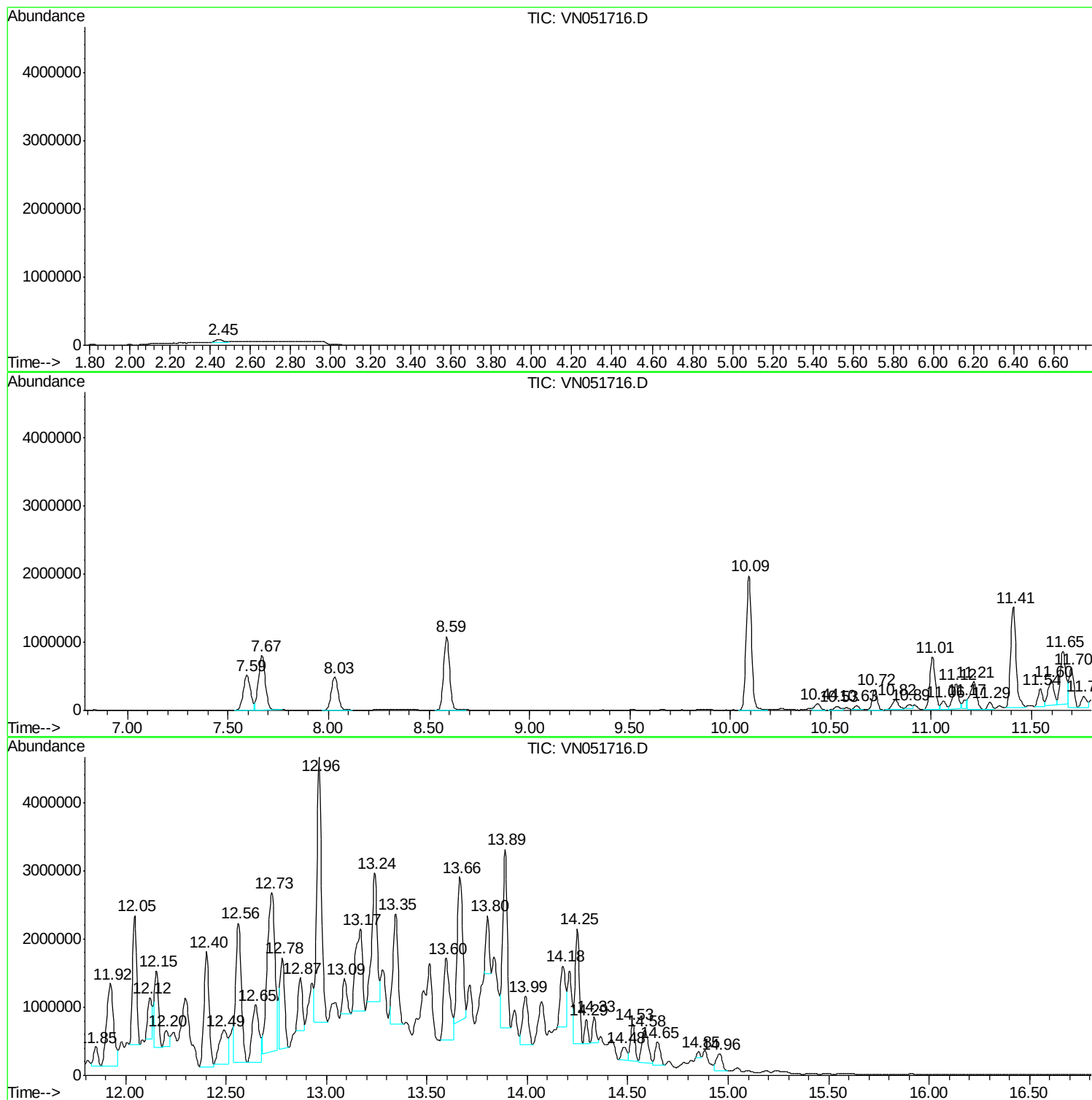
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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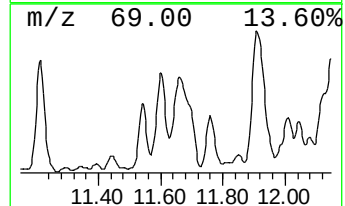
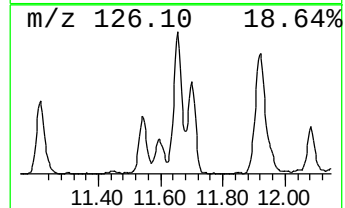
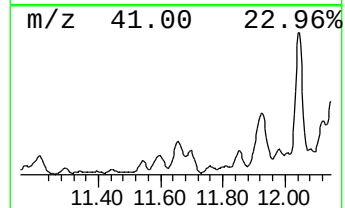
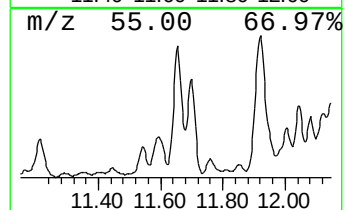
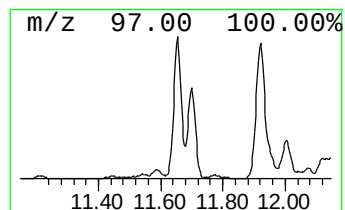
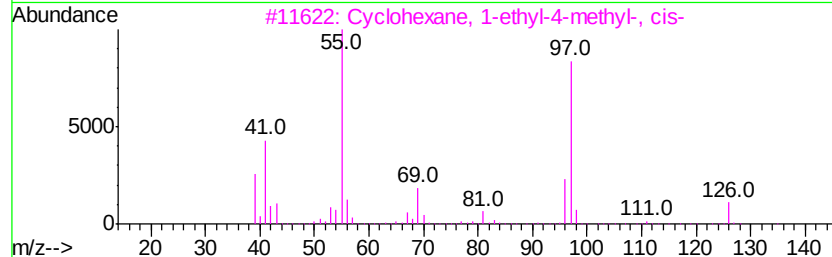
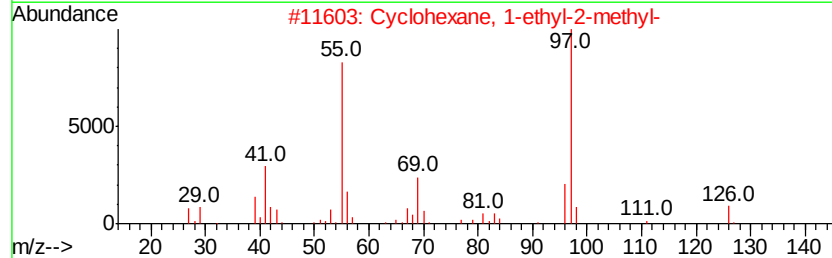
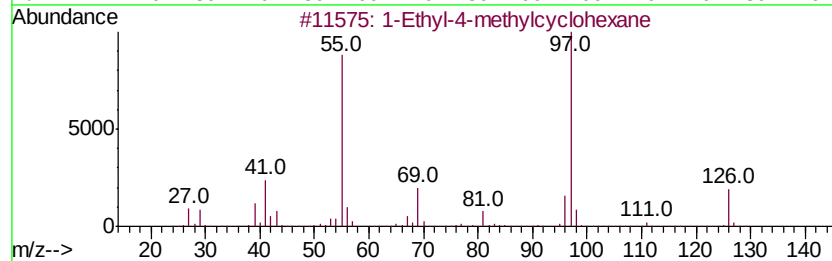
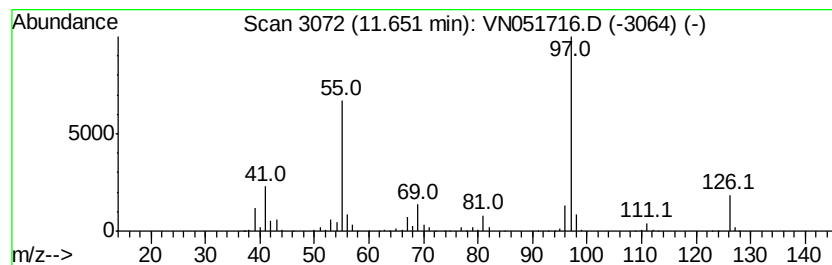
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N100418W.M
Quant Title : SW846 8260

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

Peak Number 1 1-Ethyl-4-methylcyclohexane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.65	27.52 ug/l	1511790	Chlorobenzene-d5	11.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Ethyl-4-methylcyclohexane	126	C9H18	003728-56-1	94
2		Cyclohexane, 1-ethyl-2-methyl-	126	C9H18	003728-54-9	91
3		Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	004926-78-7	87
4		Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	006236-88-0	87
5		3,5-Dimethyl-3-heptene	126	C9H18	059643-68-4	83



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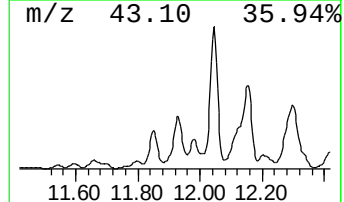
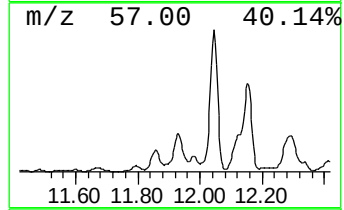
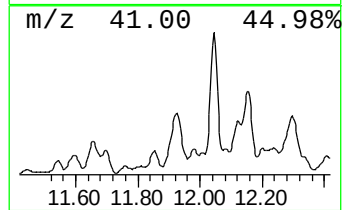
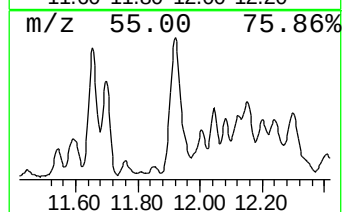
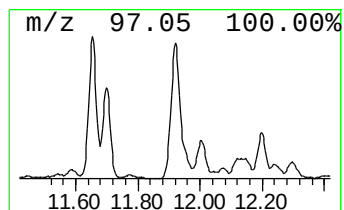
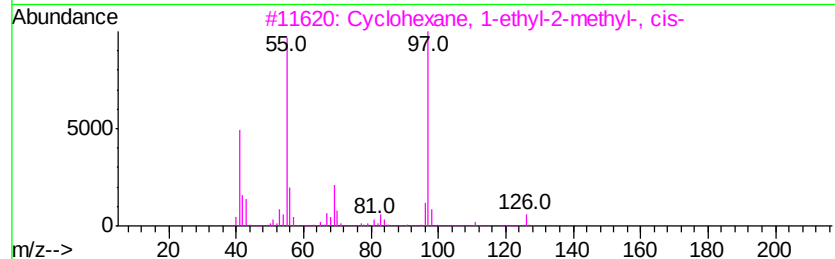
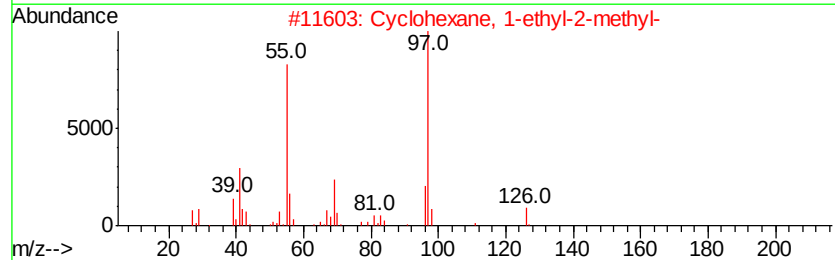
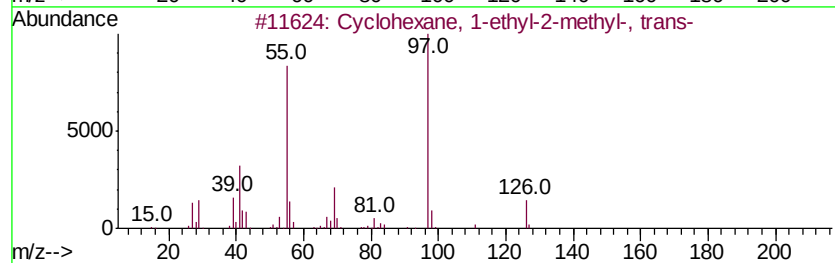
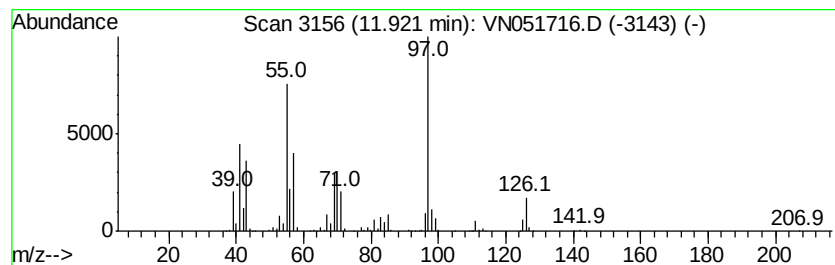
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Cyclohexane, 1-ethyl-2-meth... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	53.60 ug/l	2944440	Chlorobenzene-d5	11.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-78-8	70
2		Cyclohexane, 1-ethyl-2-methyl-	126	C9H18	003728-54-9	70
3		Cyclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-77-7	53
4		Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	006236-88-0	53
5		4-Undecen-6-one	168	C11H20O	032064-74-7	53



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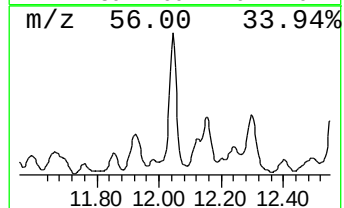
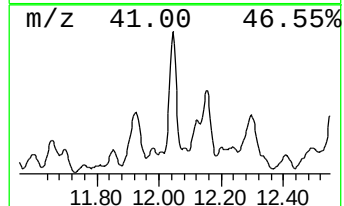
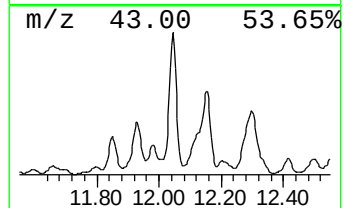
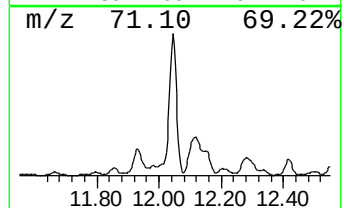
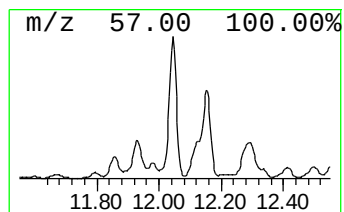
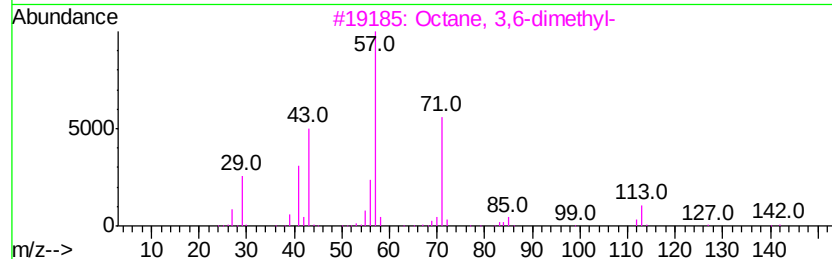
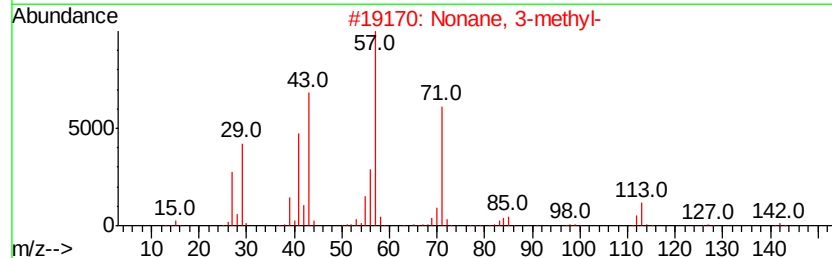
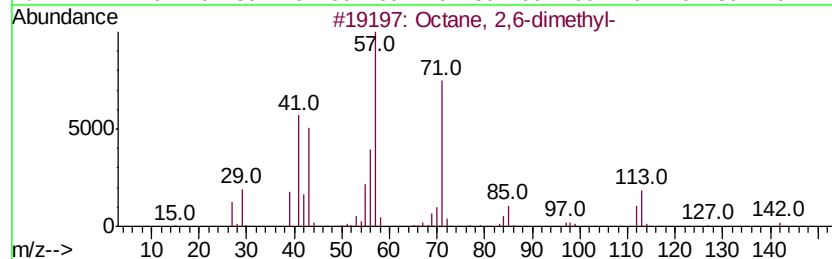
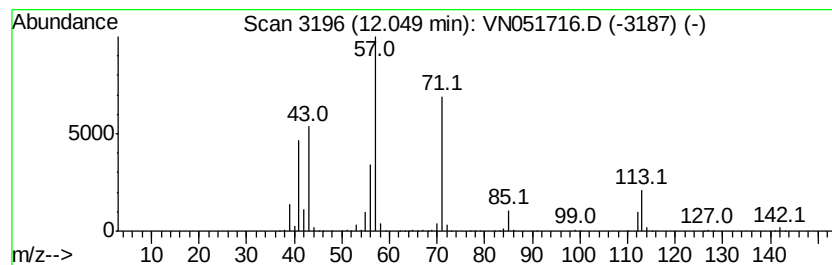
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Octane, 2,6-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.05	47.50 ug/l	2609560	Chlorobenzene-d5	11.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	90
2		Nonane, 3-methyl-	142	C10H22	005911-04-6	86
3		Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	64
4		Octane, 1,1'-oxybis-	242	C16H34O	000629-82-3	64
5		Heptane, 2,6-dimethyl-	128	C9H20	001072-05-5	53



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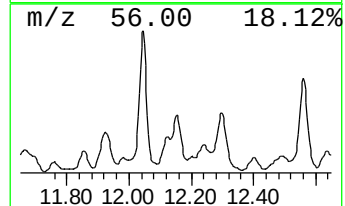
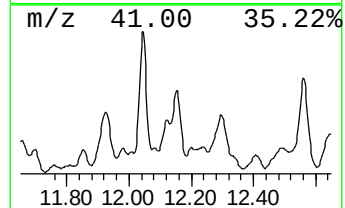
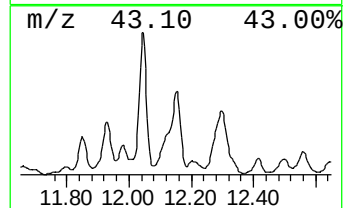
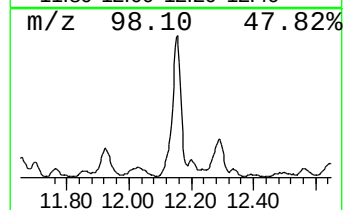
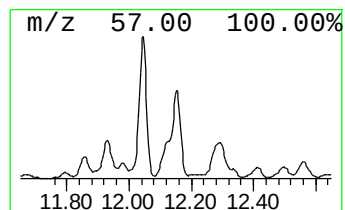
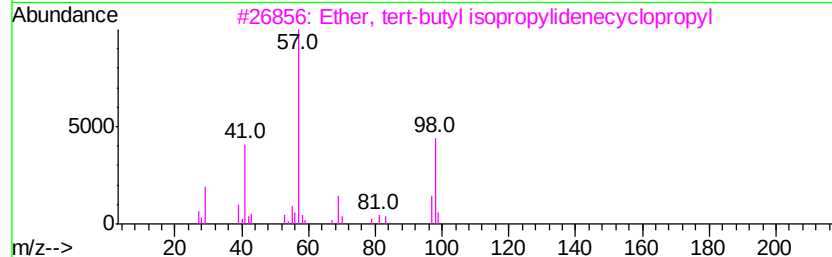
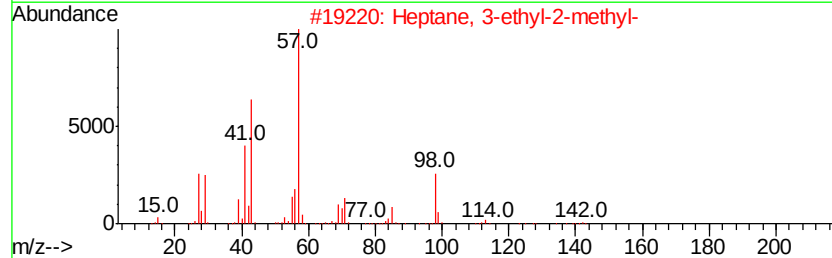
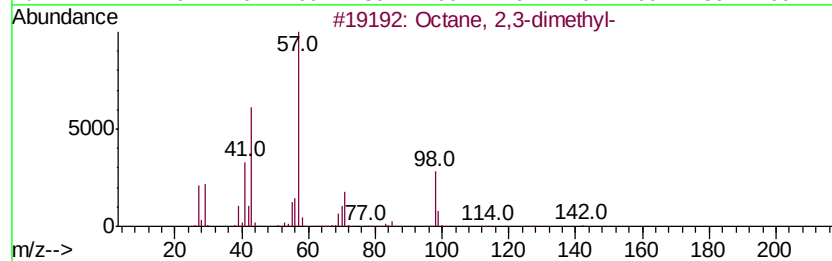
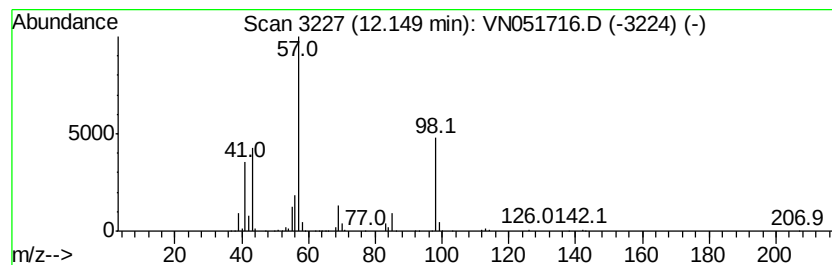
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Peak Number 4 Octane, 2,3-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.		
12.15	28.81 ug/l	1582550	Chlorobenzene-d5	11.41		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	64	
2	Heptane, 3-ethyl-2-methyl-	142	C10H22	014676-29-0	53	
3	Ether, tert-butyl isopropylidene...	154	C10H18O	024524-56-9	45	
4	Heptane, 2,3,6-trimethyl-	142	C10H22	004032-93-3	43	
5	Heptane, 4-(1-methylethyl)-	142	C10H22	052896-87-4	38	



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ALS Vial : 46 Sample Multiplier: 28

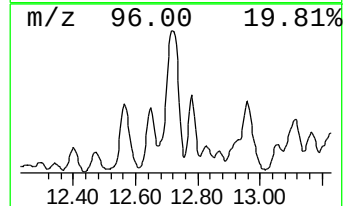
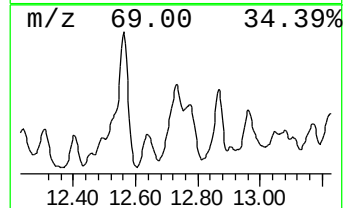
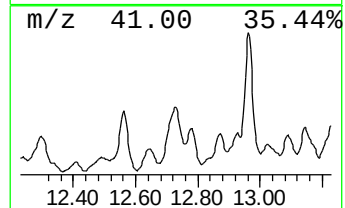
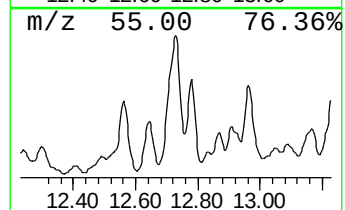
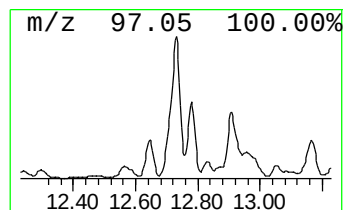
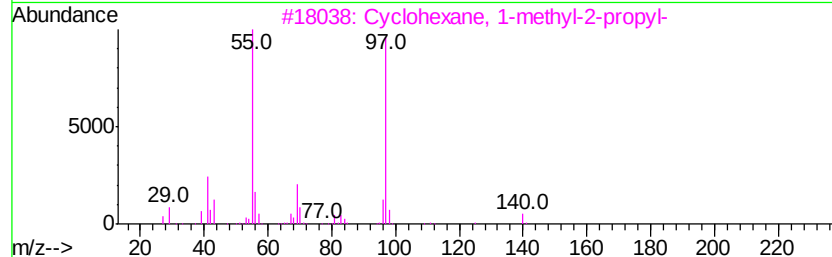
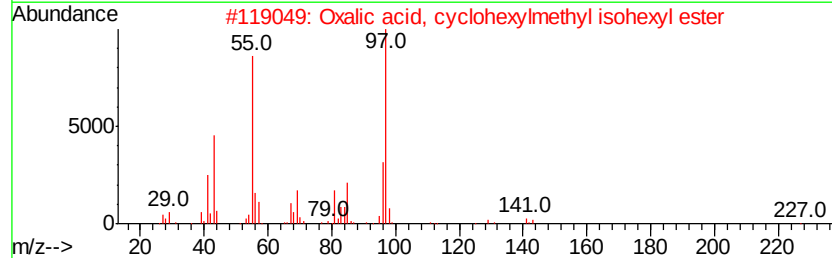
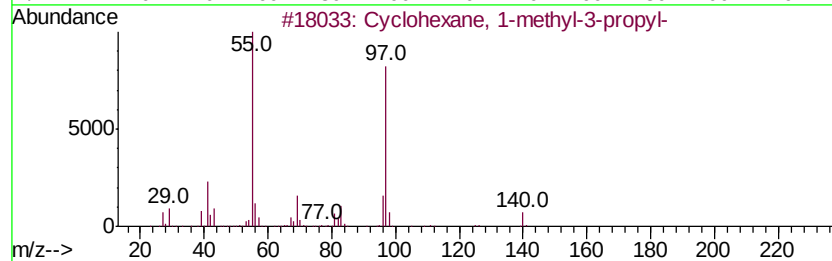
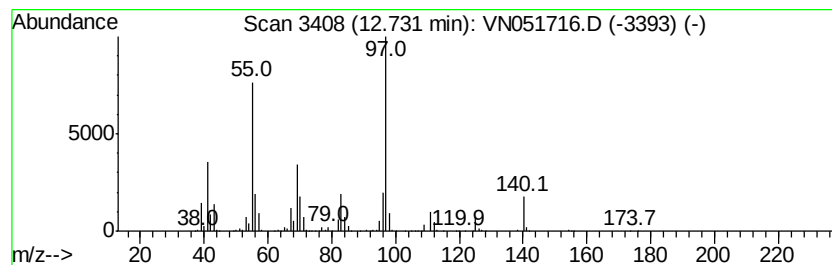
Instrument :
MSVOA_N
ClientSampleId :
EP1-MW-D-092718(7-10)

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N100418W.M
Quant Title : SW846 8260

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

Peak Number 6 Cyclohexane, 1-methyl-3-pro... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.73	106.69 ug/l	6291440	1,4-Dichlorobenzene-d4	13.35
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Cyclohexane, 1-methyl-3-propyl-	140 C10H20	004291-80-9 64
2		Oxalic acid, cyclohexylmethyl is...	270 C15H26O4	1000309-68-3 58
3		Cyclohexane, 1-methyl-2-propyl-	140 C10H20	004291-79-6 58
4		3-Hexene, 3-ethyl-2,5-dimethyl-	140 C10H20	062338-08-3 53
5		Cyclohexane, 1,1-dimethyl-	112 C8H16	000590-66-9 49



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN100618\
Data File : VN051716.D
Acq On : 6 Oct 2018 3:45
Operator : MD\SY
Sample : J5165-05 40X
Misc : 6.24g/5.00mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 46 Sample Multiplier: 28

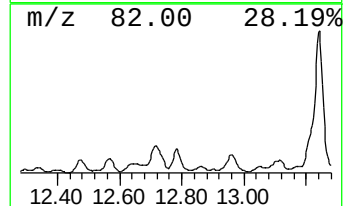
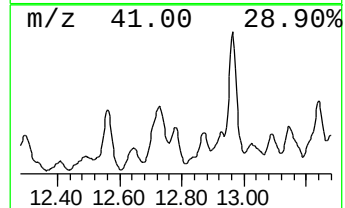
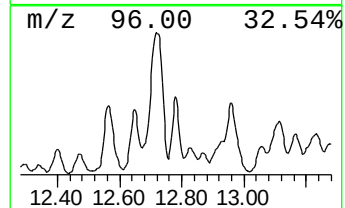
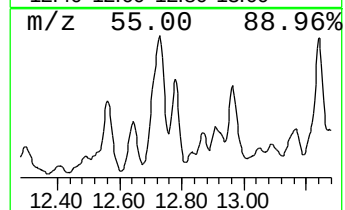
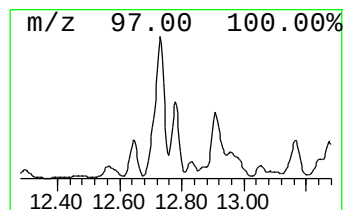
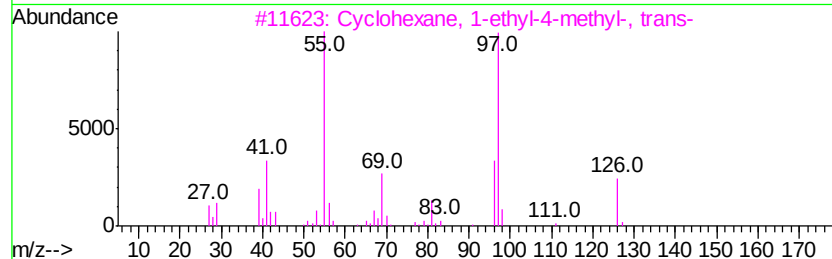
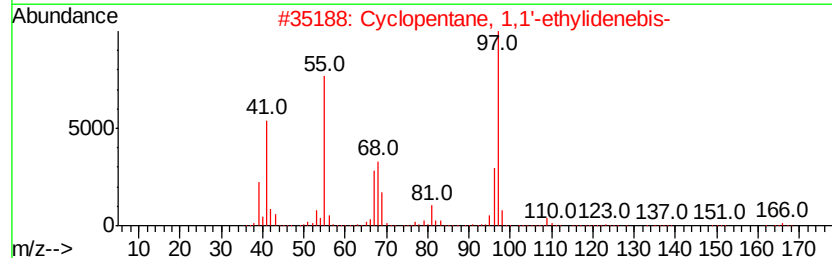
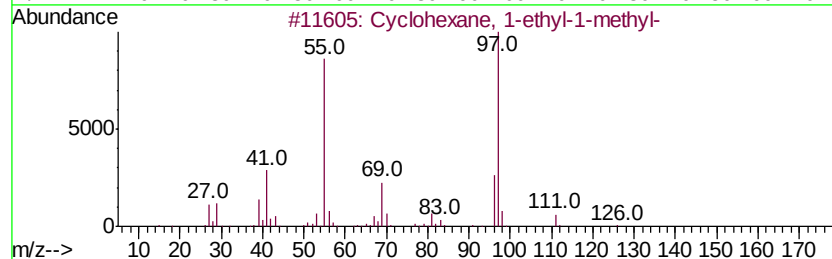
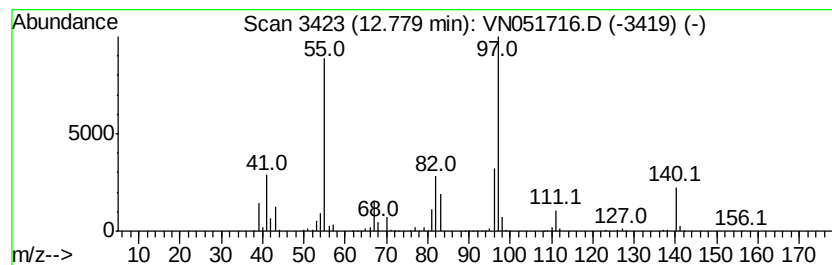
Instrument :
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ClientSampleId :
EP1-MW-D-092718(7-10)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N100418W.M
Quant Title : SW846 8260

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

Peak Number 7 Cyclohexane, 1-ethyl-1-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.78	32.96 ug/l	1943430	1,4-Dichlorobenzene-d4	13.35
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Cyclohexane, 1-ethyl-1-methyl-	126 C9H18	004926-90-3 58
2		Cyclopentane, 1,1'-ethylidenebis-	166 C12H22	004413-21-2 50
3		Cyclohexane, 1-ethyl-4-methyl-, ...	126 C9H18	006236-88-0 50
4		trans-2-Oxabicyclo[4.4.0]decane	140 C9H16O	059958-46-2 49
5		cis-2-Oxabicyclo[4.4.0]decane	140 C9H16O	060416-19-5 49



Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN100618\
Data File : VN051716.D
Acq On : 6 Oct 2018 3:45
Operator : MD\SY
Sample : J5165-05 40X
Misc : 6.24g/5.00mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 46 Sample Multiplier: 28

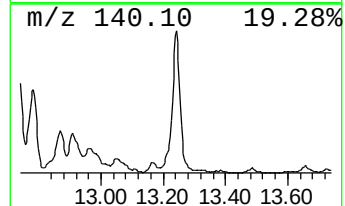
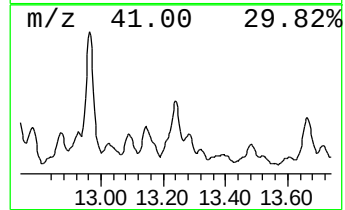
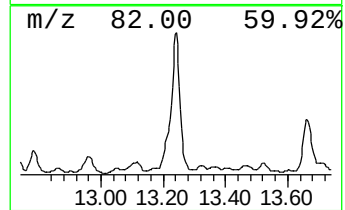
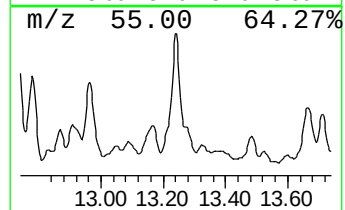
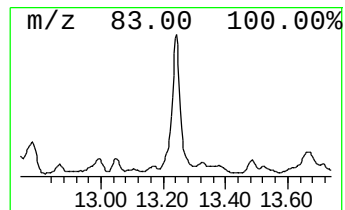
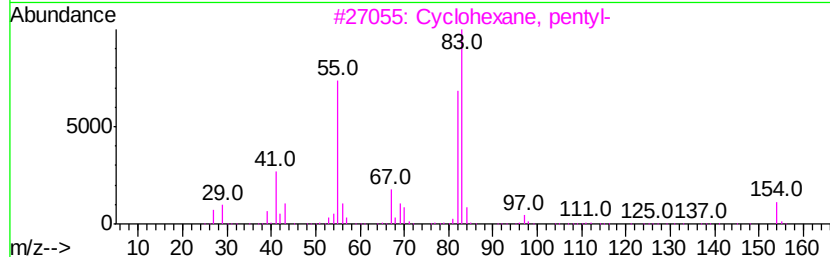
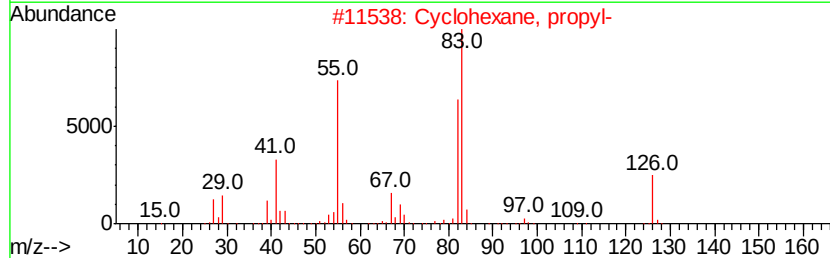
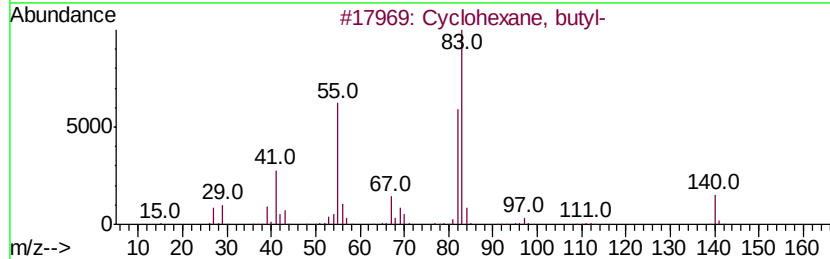
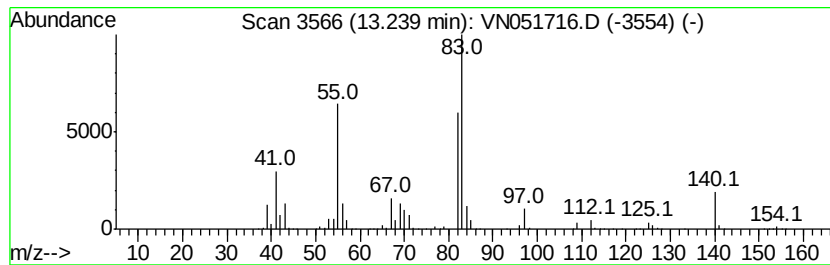
Instrument :
MSVOA_N
ClientSampleId :
EP1-MW-D-092718(7-10)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N100418W.M
Quant Title : SW846 8260

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

Peak Number 8 Cyclohexane, butyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.24	57.80 ug/l	3408450	1,4-Dichlorobenzene-d4	13.35
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Cyclohexane, butyl-	140 C10H20	001678-93-9 93
2		Cyclohexane, propyl-	126 C9H18	001678-92-8 76
3		Cyclohexane, pentyl-	154 C11H22	004292-92-6 74
4		Cyclohexane, undecyl-	238 C17H34	054105-66-7 72
5		Cyclohexane, ethyl-	112 C8H16	001678-91-7 68



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN100618\
Data File : VN051716.D
Acq On : 6 Oct 2018 3:45
Operator : MD\SY
Sample : J5165-05 40X
Misc : 6.24µ/5.00mL/100µL/5.00mL/MSVOA_N/MEOH
ALS Vial : 46 Sample Multiplier: 28

Instrument :
MSVOA_N
ClientSampleId :
EP1-MW-D-092718(7-10)

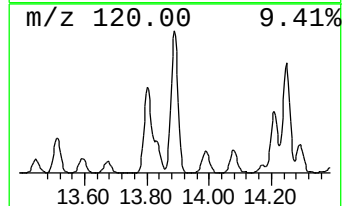
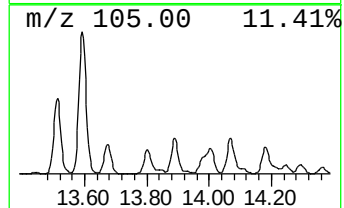
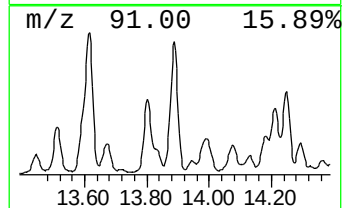
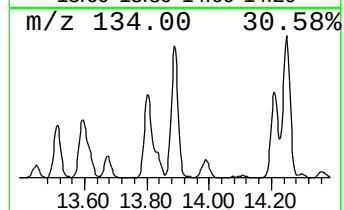
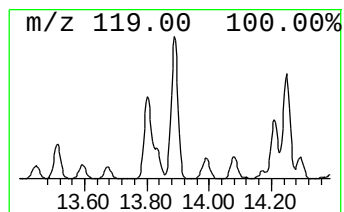
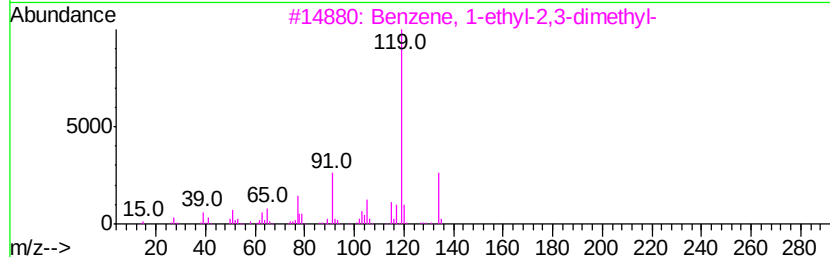
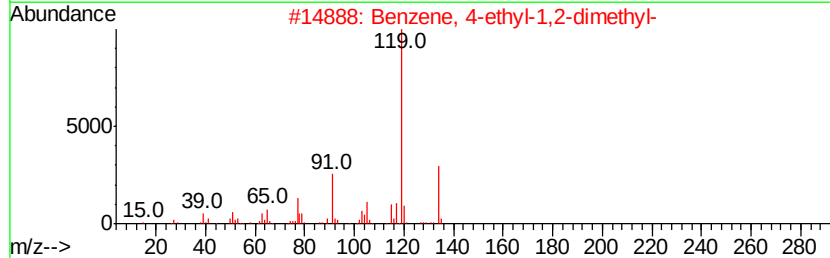
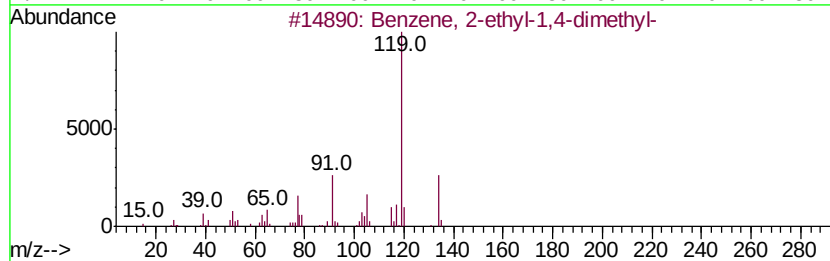
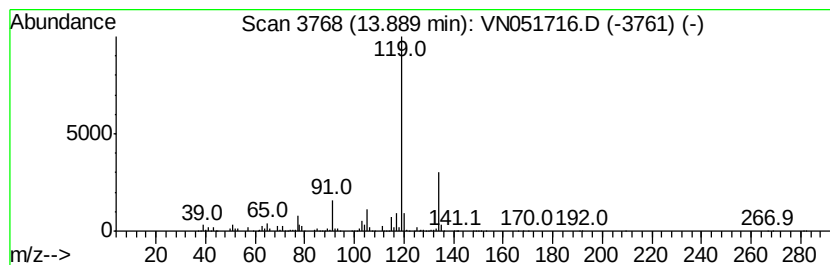
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Quant Title : SW846 8260

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

Peak Number 9 Benzene, 2-ethyl-1,4-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	67.62 ug/l	3987590	1,4-Dichlorobenzene-d4	13.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	96
2		Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	95
3		Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95
4		Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	94
5		Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	94



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN100618\
Data File : VN051716.D
Acq On : 6 Oct 2018 3:45
Operator : MD\SY
Sample : J5165-05 40X
Misc : 6.24g/5.00mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 46 Sample Multiplier: 28

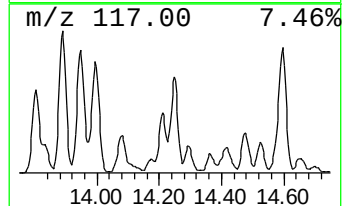
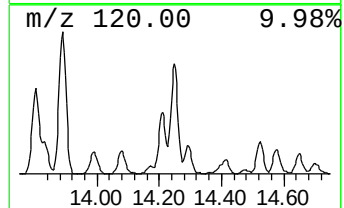
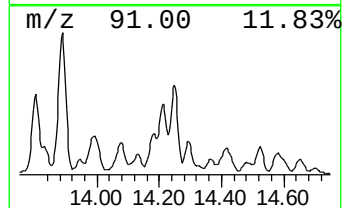
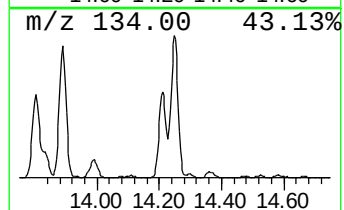
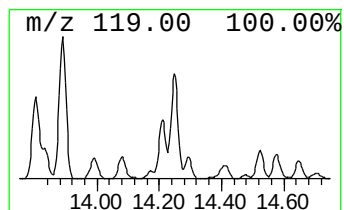
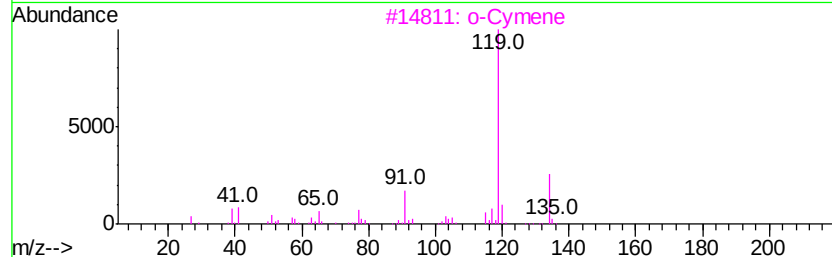
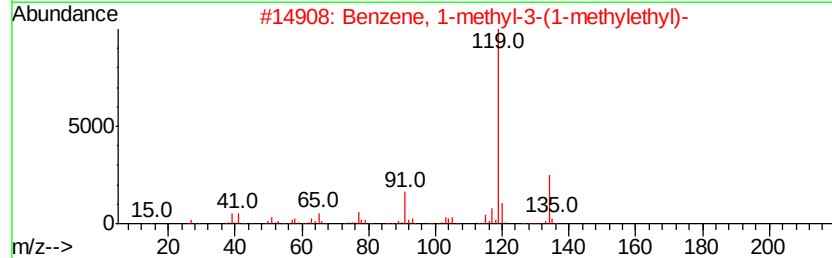
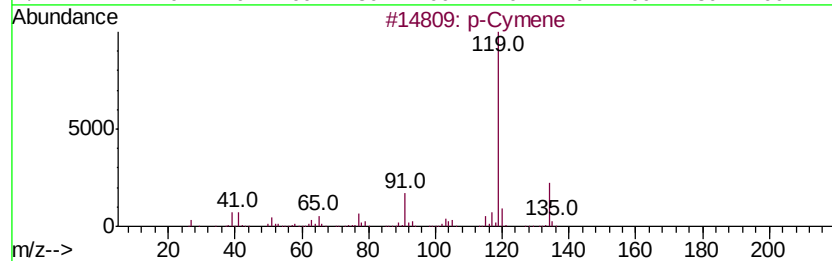
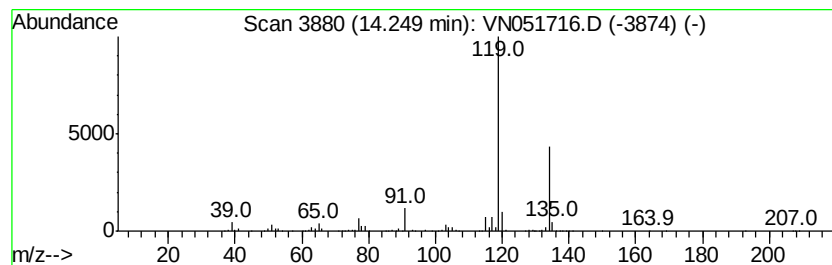
Instrument :
MSVOA_N
ClientSampleId :
EP1-MW-D-092718(7-10)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N100418W.M
Quant Title : SW846 8260

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

Peak Number 10 p-Cymene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.25	41.09 ug/l	2423290	1,4-Dichlorobenzene-d4	13.35
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	p-Cymene		134 C10H14	000099-87-6 95
2	Benzene, 1-methyl-3-(1-methyleth...		134 C10H14	000535-77-3 95
3	o-Cymene		134 C10H14	000527-84-4 94
4	Benzene, 1-ethyl-3,5-dimethyl-		134 C10H14	000934-74-7 91
5	Benzene, 2-ethyl-1,3-dimethyl-		134 C10H14	002870-04-4 91



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN100618\
Data File : VN051716.D
Acq On : 6 Oct 2018 3:45
Operator : MD\SY
Sample : J5165-05 40X
Misc : 6.24g/5.00mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 46 Sample Multiplier: 28

Instrument :
MSVOA_N
ClientSampleId :
EP1-MW-D-092718(7-10)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N100418W.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
1-Ethyl-4-methylc...	11.65	27.5	ug/l	1511790	3	11.41	2746900	50.0
Cyclohexane, 1-et...	11.92	53.6	ug/l	2944440	3	11.41	2746900	50.0
Octane, 2,6-dimet...	12.05	47.5	ug/l	2609560	3	11.41	2746900	50.0
Octane, 2,3-dimet...	12.15	28.8	ug/l	1582550	3	11.41	2746900	50.0
unknown12.65	12.65	33.9	ug/l	1999970	4	13.35	2948490	50.0
Cyclohexane, 1-me...	12.73	106.7	ug/l	6291440	4	13.35	2948490	50.0
Cyclohexane, 1-et...	12.78	33.0	ug/l	1943430	4	13.35	2948490	50.0
Cyclohexane, butyl-	13.24	57.8	ug/l	3408450	4	13.35	2948490	50.0
Benzene, 2-ethyl-...	13.89	67.6	ug/l	3987590	4	13.35	2948490	50.0
p-Cymene	14.25	41.1	ug/l	2423290	4	13.35	2948490	50.0