

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN052119\
 Data File : VN055718.D
 Acq On : 21 May 2019 18:43
 Operator : JC/SP
 Sample : K2977-04 50X
 Misc : 5.61g/5mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 EP1-W-2R(17-20)

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\82N051719W.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	1790	1809	1820	rBV	231612	570800	8.17%	0.916%
2	7.667	1820	1833	1872	rVB	435798	1062774	15.22%	1.705%
3	8.027	1928	1945	1966	rBV	212099	495228	7.09%	0.795%
4	8.217	1979	2004	2038	rBV3	33043	183513	2.63%	0.294%
5	8.587	2102	2119	2169	rVB	571946	1236459	17.70%	1.984%
6	10.091	2572	2587	2617	rVB	908631	1811158	25.93%	2.906%
7	10.432	2684	2693	2712	rVB	43877	83213	1.19%	0.134%
8	10.718	2771	2782	2795	rVB	73235	126022	1.80%	0.202%
9	10.818	2795	2813	2826	rBV	60503	132940	1.90%	0.213%
10	10.953	2846	2855	2862	rBV	107257	162082	2.32%	0.260%
11	11.004	2862	2871	2882	rVB	197724	343003	4.91%	0.550%
12	11.123	2896	2908	2916	rBV3	152612	278206	3.98%	0.446%
13	11.207	2916	2934	2950	rVB5	236746	698944	10.01%	1.121%
14	11.297	2950	2962	2982	rBV	258176	498011	7.13%	0.799%
15	11.406	2983	2996	3014	rBV	791372	1486807	21.29%	2.385%
16	11.490	3014	3022	3029	rBV3	42581	79927	1.14%	0.128%
17	11.541	3030	3038	3045	rBV	125717	190864	2.73%	0.306%
18	11.596	3045	3055	3061	rBV6	204116	434198	6.22%	0.697%
19	11.654	3065	3073	3081	rVV2	535145	875264	12.53%	1.404%
20	11.696	3082	3086	3097	rVB2	467101	703840	10.08%	1.129%
21	11.757	3097	3105	3111	rBV3	107883	190663	2.73%	0.306%
22	11.811	3112	3122	3126	rBV2	82329	154320	2.21%	0.248%
23	11.850	3127	3134	3142	rVB3	308339	474771	6.80%	0.762%
24	11.924	3143	3157	3168	rBV6	1056162	2542681	36.40%	4.079%
25	12.043	3187	3194	3202	rVB	1299005	1744223	24.97%	2.798%
26	12.120	3210	3218	3223	rBV3	825168	1331058	19.06%	2.135%
27	12.162	3224	3231	3249	rVB4	1659623	3150677	45.11%	5.055%
28	12.294	3265	3272	3279	rBV6	515912	909086	13.02%	1.458%
29	12.336	3280	3285	3295	rVB2	1307180	1953619	27.97%	3.134%
30	12.403	3295	3306	3316	rBV4	933538	1750836	25.07%	2.809%
31	12.487	3317	3332	3339	rBV8	390349	1090409	15.61%	1.749%
32	12.561	3348	3355	3371	rVB3	1191192	2734712	39.15%	4.387%
33	12.644	3371	3381	3387	rBV7	553343	1081143	15.48%	1.735%
34	12.728	3388	3407	3416	rVV5	1626109	5344275	76.51%	8.574%

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35	12.779	3417	3423	3433	rVB4	850739	1416320	20.28%	2.272%
36	12.869	3444	3451	3458	rBV6	484840	666986	9.55%	1.070%
37	12.959	3472	3479	3492	rVB2	1971458	3308280	47.36%	5.308%
38	13.040	3493	3504	3513	rBV	4322939	6984784	100.00%	11.206%
39	13.165	3532	3543	3551	rVB6	530190	1252984	17.94%	2.010%
40	13.239	3552	3566	3573	rBV3	1276160	2493458	35.70%	4.000%
41	13.284	3575	3580	3588	rVB3	686860	966858	13.84%	1.551%
42	13.342	3592	3598	3605	rBV	414933	565772	8.10%	0.908%
43	13.593	3668	3676	3688	rBV3	459690	1027464	14.71%	1.648%
44	13.660	3689	3697	3707	rVV4	1063774	1978956	28.33%	3.175%
45	13.709	3708	3712	3721	rVB2	267748	363691	5.21%	0.583%
46	13.799	3736	3740	3745	rBV3	222688	309046	4.42%	0.496%
47	13.831	3746	3750	3760	rVV4	545784	780667	11.18%	1.252%
48	13.885	3761	3767	3776	rVB	682970	1042779	14.93%	1.673%
49	13.991	3791	3800	3809	rVB5	372258	629824	9.02%	1.010%
50	14.178	3849	3858	3873	rVV6	312988	859091	12.30%	1.378%
51	14.245	3874	3879	3887	rVB	321001	438257	6.27%	0.703%
52	14.294	3888	3894	3899	rBV3	99131	128585	1.84%	0.206%
53	14.329	3900	3905	3913	rVB4	151407	194139	2.78%	0.311%
54	14.480	3944	3952	3959	rBV5	45586	99898	1.43%	0.160%
55	14.522	3961	3965	3973	rVV3	93946	123383	1.77%	0.198%
56	14.580	3973	3983	3995	rVV2	336913	647081	9.26%	1.038%
57	14.644	3996	4003	4014	rVB3	86662	146593	2.10%	0.235%

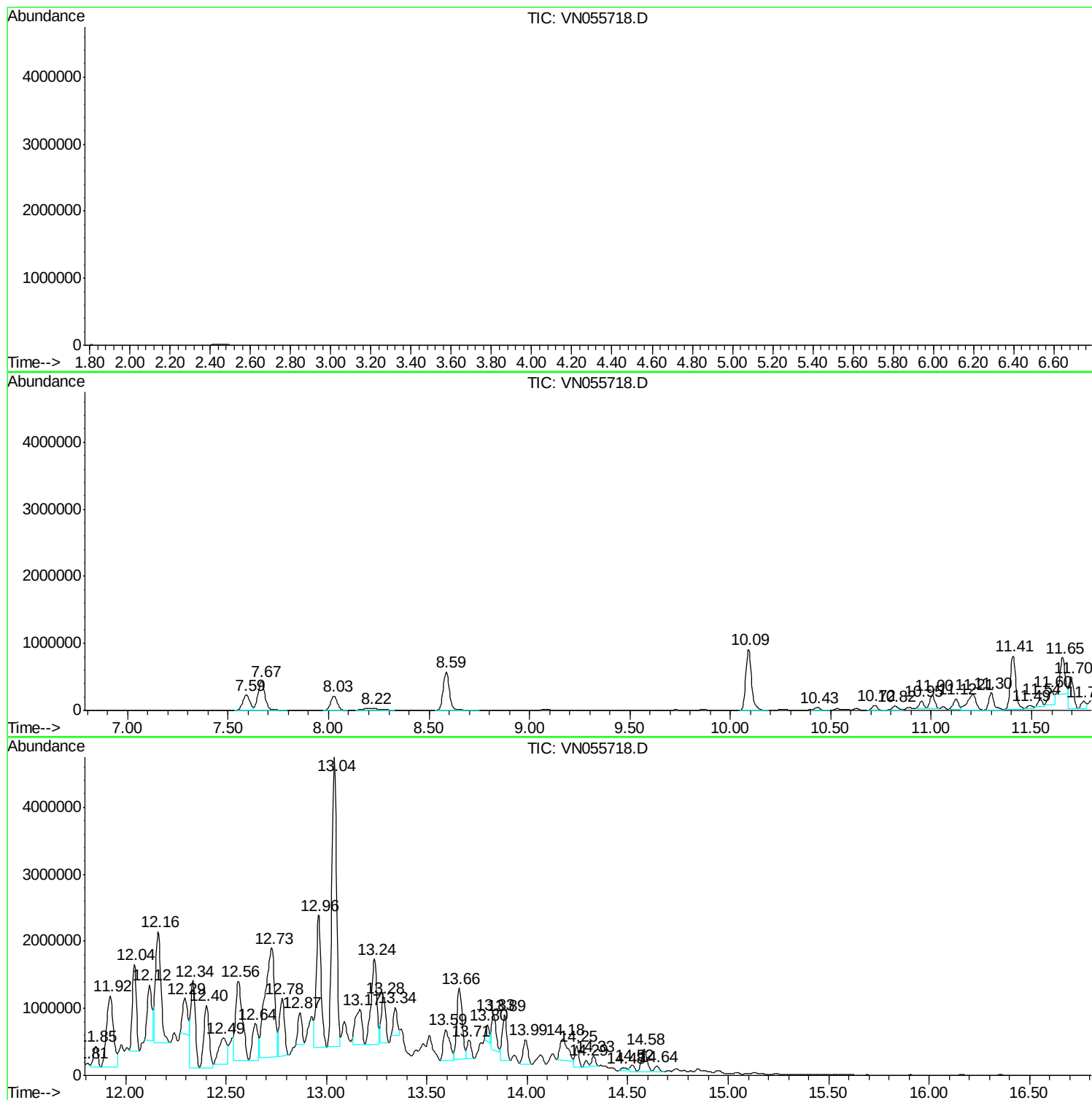
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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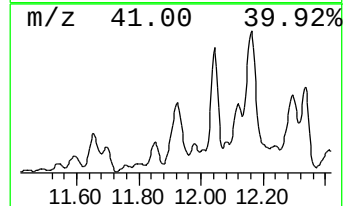
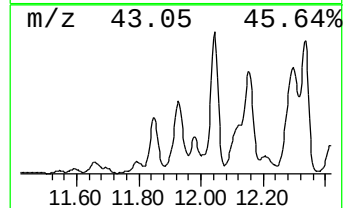
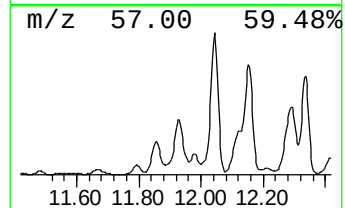
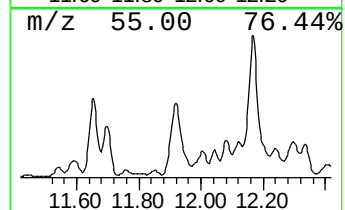
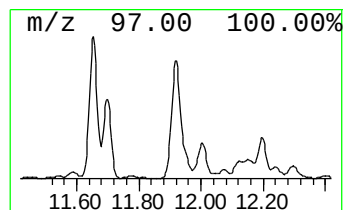
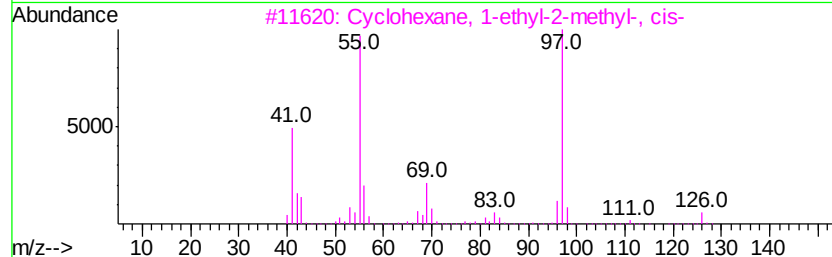
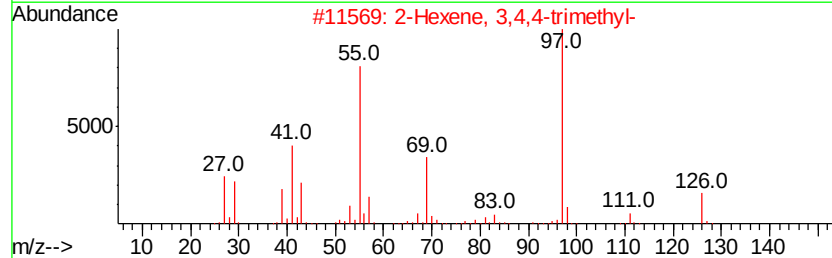
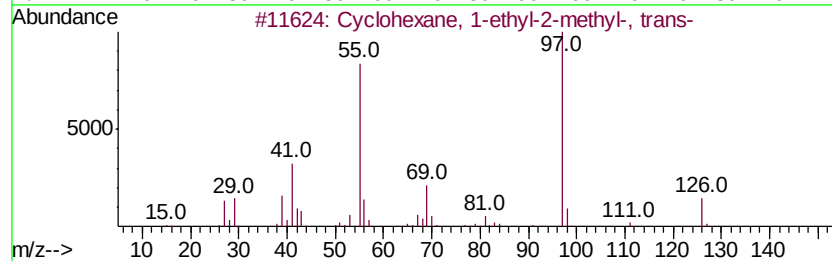
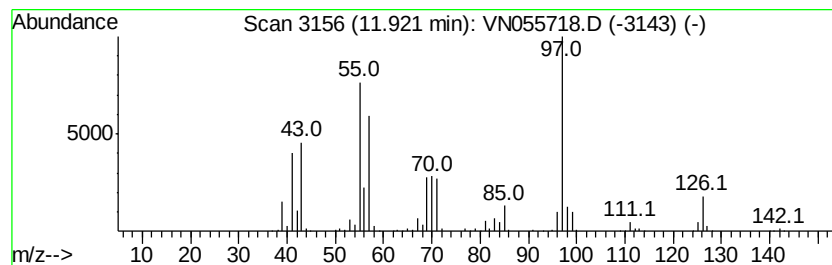
Instrument :
MSVOA_N
ClientSampled :
EP1-W-2R(17-20)

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N051719W.M
Quant Title : SW846 8260

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

Peak Number 1 Cyclohexane, 1-ethyl-2-meth... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.		
11.92	85.51 ug/l	2542680	Chlorobenzene-d5	11.41		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-78-8	55
2		2-Hexene, 3,4,4-trimethyl-	126	C9H18	053941-19-8	46
3		Cyclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-77-7	43
4		1-Ethyl-3-methylcyclohexane (c,t)	126	C9H18	003728-55-0	43
5		1-Ethyl-4-methylcyclohexane	126	C9H18	003728-56-1	43



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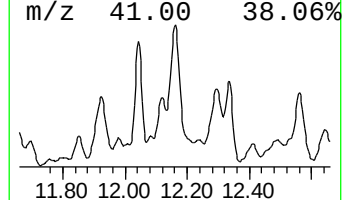
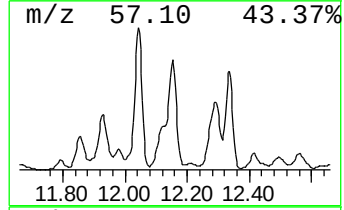
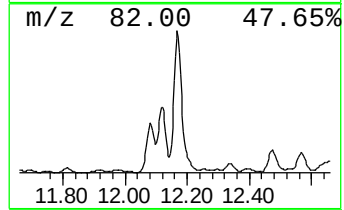
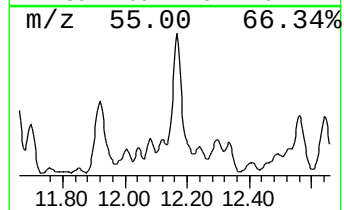
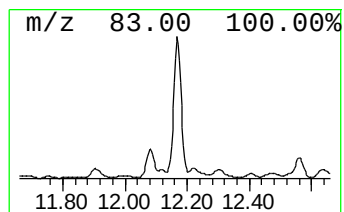
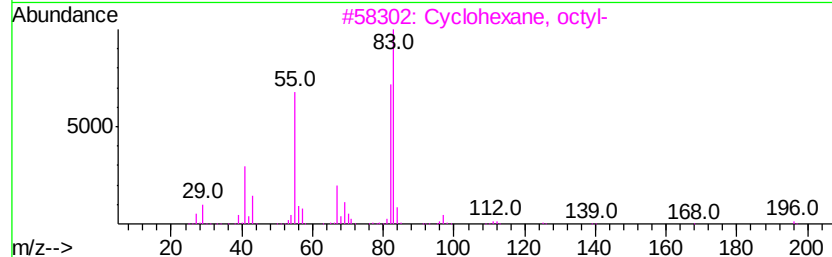
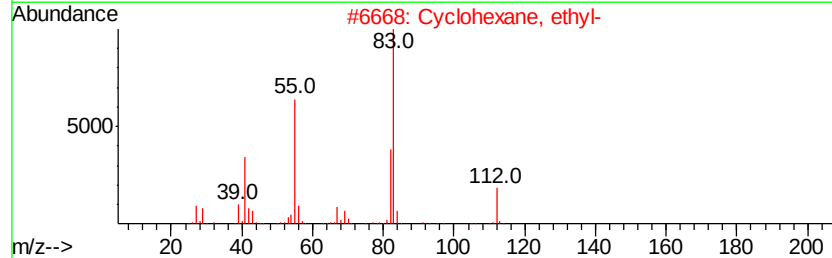
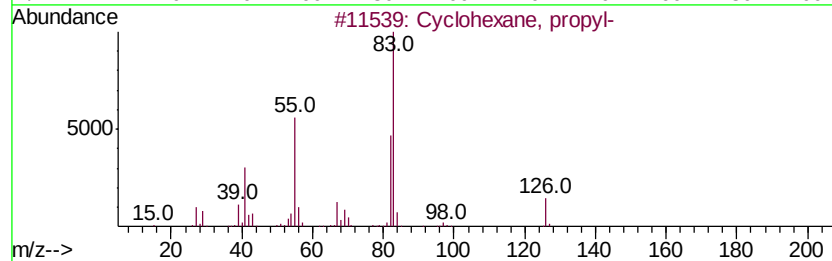
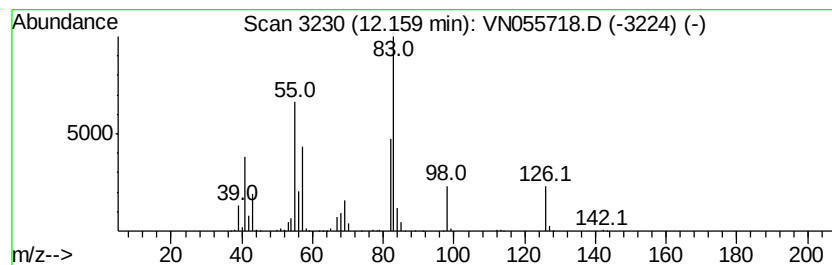
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Cyclohexane, propyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.		
12.16	105.95 ug/l	3150680	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	64
3		Cyclohexane, octyl-	196	C14H28	001795-15-9	64
4		Cyclopentane, 1-ethyl-1-methyl-	112	C8H16	016747-50-5	53
5		2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	52



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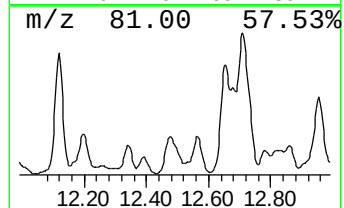
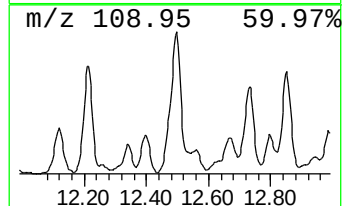
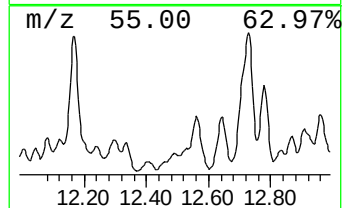
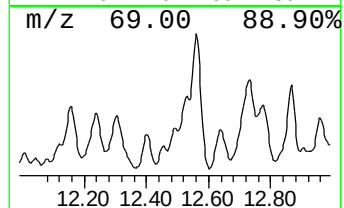
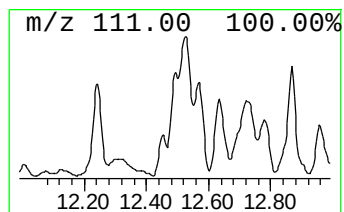
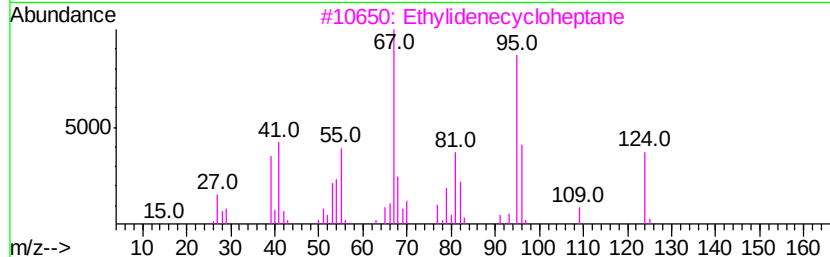
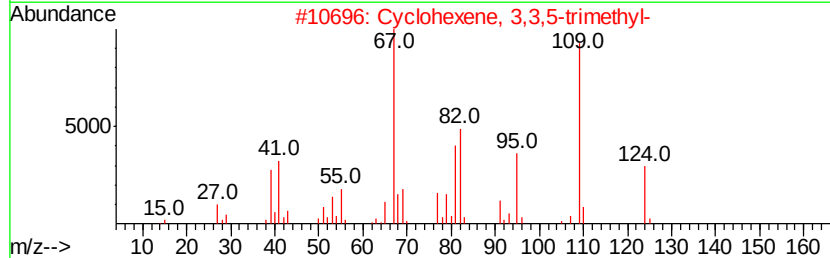
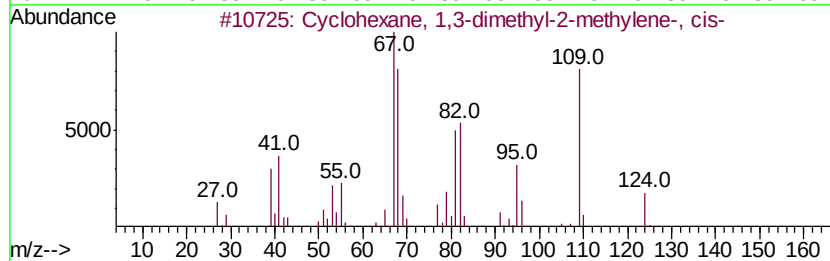
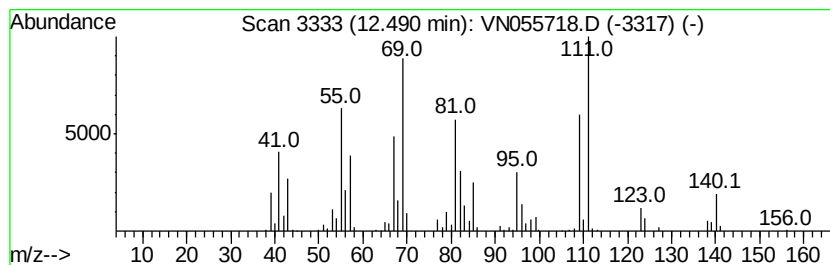
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown12.49 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.49	96.36 ug/l	1090410	1,4-Dichlorobenzene-d4	13.34	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,3-dimethyl-2-meth...	124	C9H16	019781-47-6	42
2	Cyclohexene, 3,3,5-trimethyl-	124	C9H16	000503-45-7	41
3	Ethylidenecycloheptane	124	C9H16	010494-87-8	35
4	9-Octadecyne	250	C18H34	035365-59-4	30
5	1-Tetradecyne	194	C14H26	000765-10-6	30



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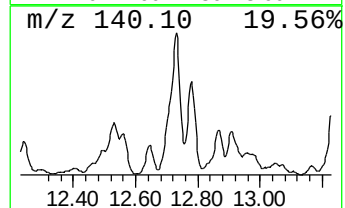
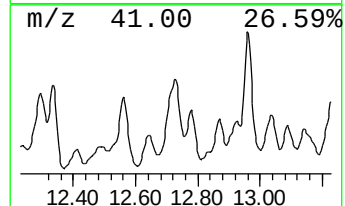
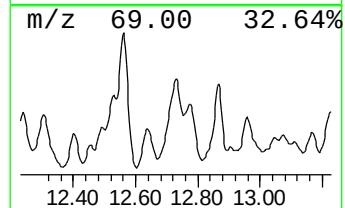
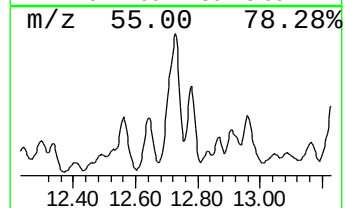
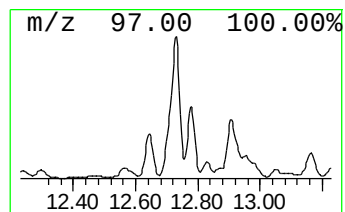
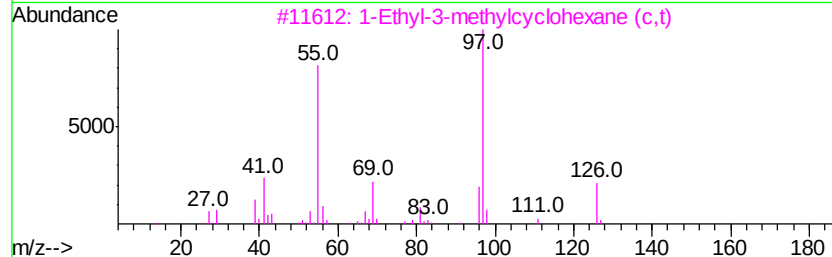
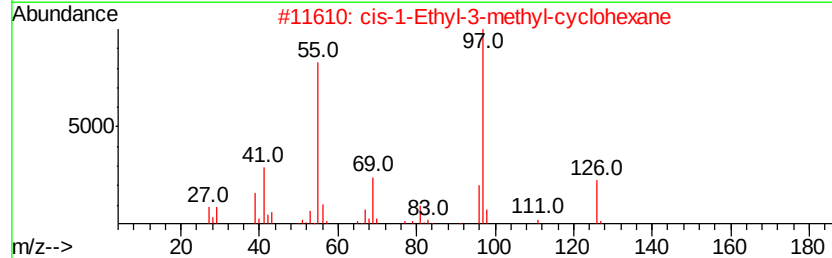
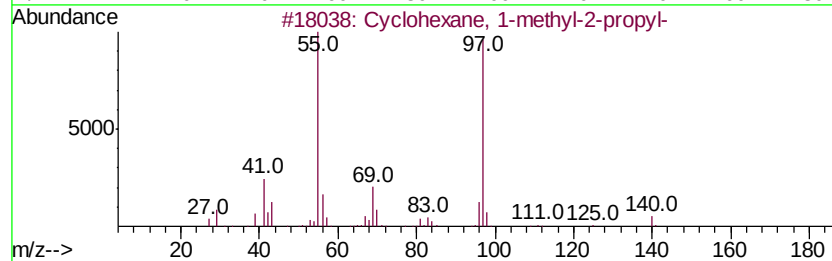
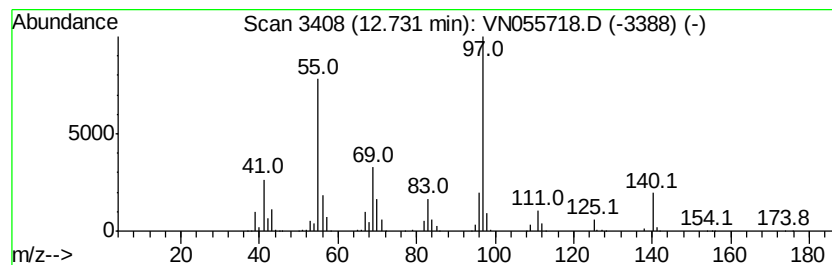
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Peak Number 5 Cyclohexane, 1-methyl-2-pro... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.73	472.30 ug/l	5344280	1,4-Dichlorobenzene-d4	13.34
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Cyclohexane, 1-methyl-2-propyl-	140 C10H20	004291-79-6 64
2		cis-1-Ethyl-3-methyl-cyclohexane	126 C9H18	019489-10-2 59
3		1-Ethyl-3-methylcyclohexane (c,t)	126 C9H18	003728-55-0 59
4		Sulfurous acid, cyclohexylmethyl...	402 C23H46O3S	1000309-22-4 53
5		2,4-Dimethyl-1,5-diazabicyclo[3....	112 C6H12N2	100463-01-2 52



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ALS Vial : 24 Sample Multiplier: 1

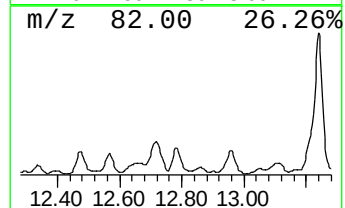
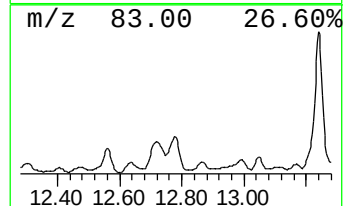
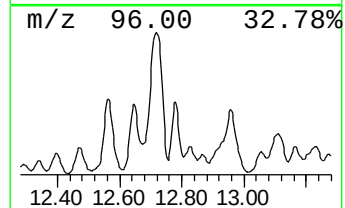
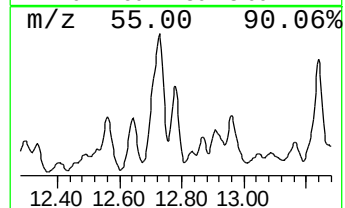
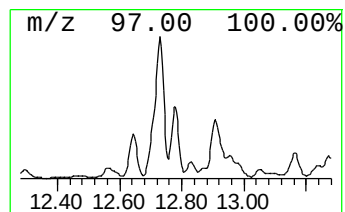
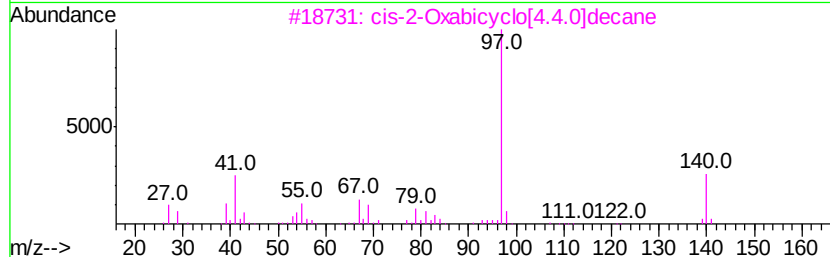
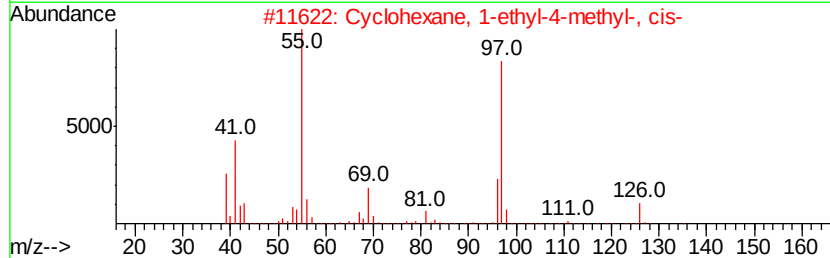
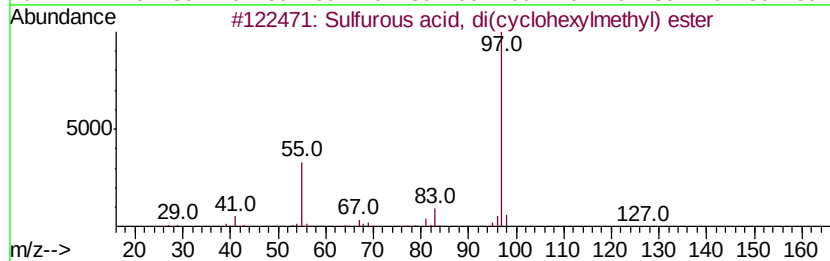
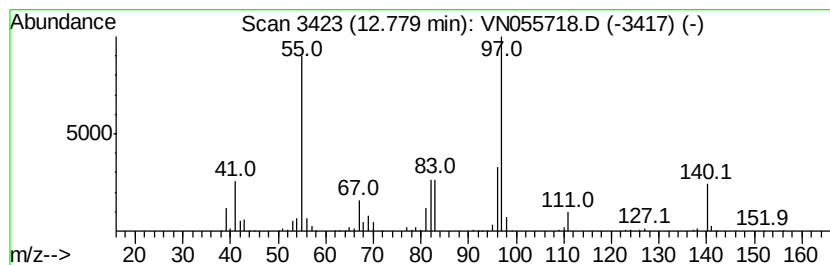
Instrument :
MSVOA_N
ClientSampleId :
EP1-W-2R(17-20)

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N051719W.M
Quant Title : SW846 8260

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

Peak Number 6 Sulfurous acid, di(cyclohex... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.		
12.78	125.17 ug/l	1416320	1,4-Dichlorobenzene-d4	13.34		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Sulfurous acid, di(cvclohexylmet...	274	C14H26O3S	1000309-22-7	52
2		Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	004926-78-7	50
3		cis-2-Oxabicyclo[4.4.0]decane	140	C9H16O	060416-19-5	49
4		Ethanone, 1-(1-methylcyclohexyl)-	140	C9H16O	002890-62-2	47
5		Sulfurous acid, cyclohexylmethyl...	262	C13H26O3S	1000309-21-6	47



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_N\DATA\VN052119\
Data File : VN055718.D
Acq On : 21 May 2019 18:43
Operator : JC/SP
Sample : K2977-04 50X
Misc : 5.61µ/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 24 Sample Multiplier: 1

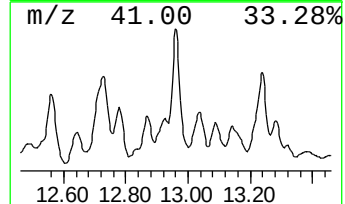
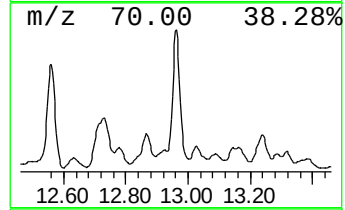
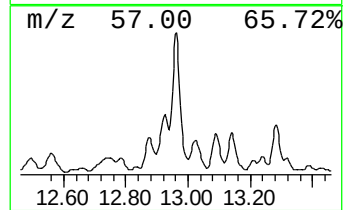
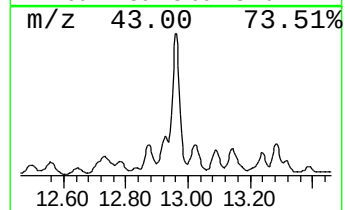
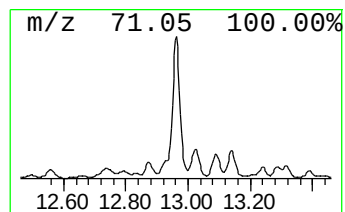
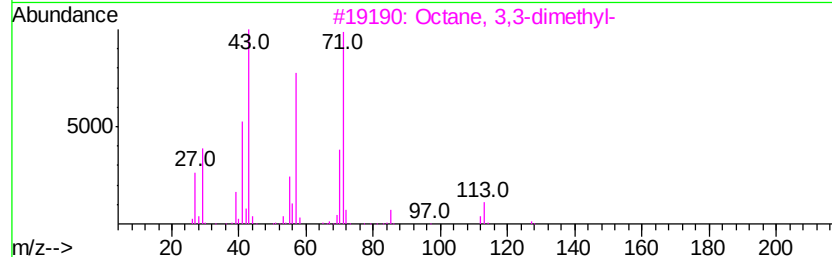
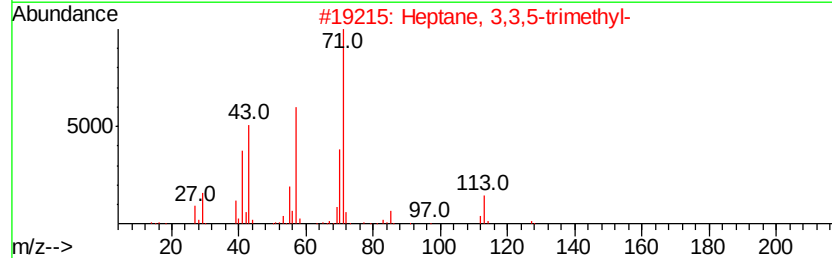
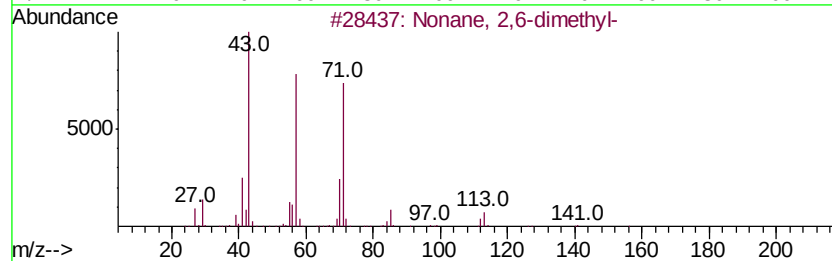
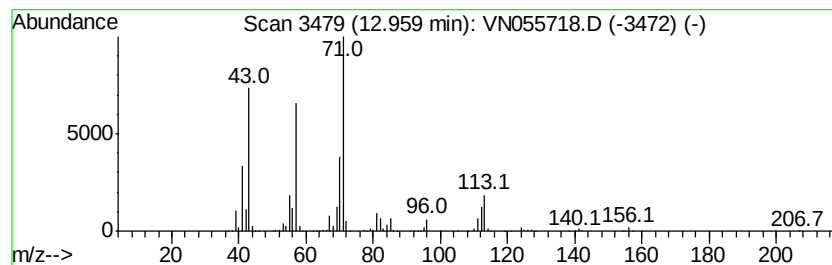
Instrument :
MSVOA_N
ClientSampleId :
EP1-W-2R(17-20)

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N051719W.M
Quant Title : SW846 8260

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

Peak Number 7 Nonane, 2,6-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.96	292.37 ug/l	3308280	1,4-Dichlorobenzene-d4	13.34
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Nonane, 2,6-dimethyl-	156 C11H24	017302-28-2 83
2		Heptane, 3,3,5-trimethyl-	142 C10H22	007154-80-5 80
3		Octane, 3,3-dimethyl-	142 C10H22	004110-44-5 64
4		2,2'-Bifuran, octahydro-	142 C8H14O2	001592-33-2 59
5		Decane, 2,3,4-trimethyl-	184 C13H28	062238-15-7 59



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_N\DATA\VN052119\
Data File : VN055718.D
Acq On : 21 May 2019 18:43
Operator : JC/SP
Sample : K2977-04 50X
Misc : 5.61µ/5mL/100µL/5.00mL/MSVOA_N/MEOH
ALS Vial : 24 Sample Multiplier: 1

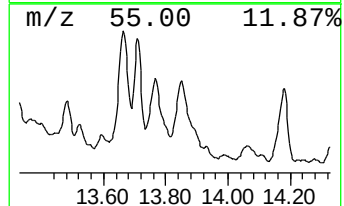
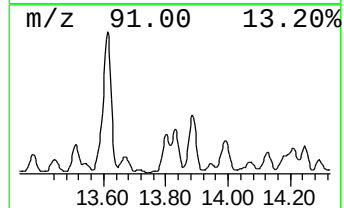
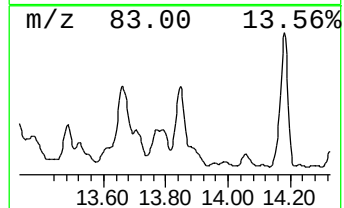
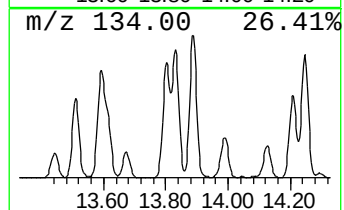
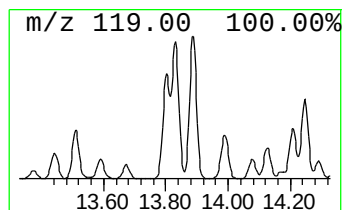
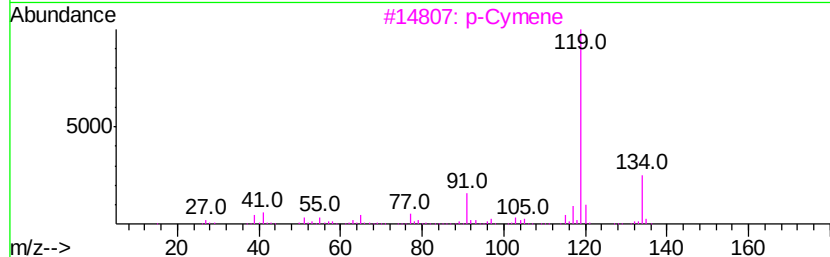
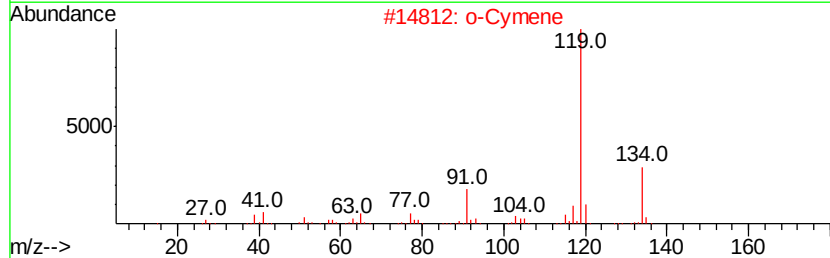
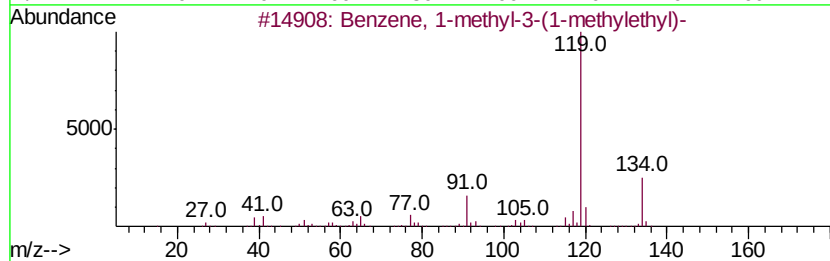
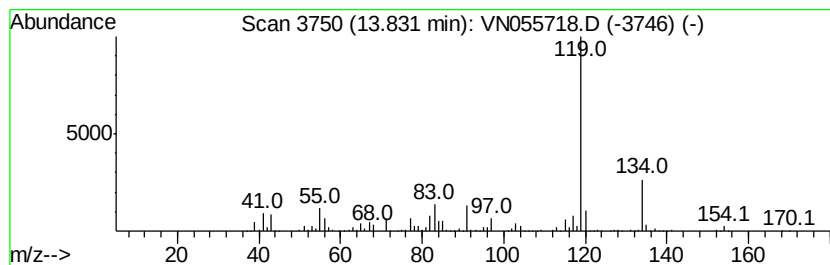
Instrument :
MSVOA_N
ClientSampled :
EP1-W-2R(17-20)

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N051719W.M
Quant Title : SW846 8260

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

Peak Number 8 Benzene, 1-methyl-3-(1-meth... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.83	68.99 ug/l	780667	1,4-Dichlorobenzene-d4	13.34	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	94
2	o-Cymene	134	C10H14	000527-84-4	93
3	p-Cymene	134	C10H14	000099-87-6	87
4	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	81
5	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	81



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA N\DATA\VN052119\
Data File : VN055718.D
Acq On : 21 May 2019 18:43
Operator : JC/SP
Sample : K2977-04 50X
Misc : 5.61µ/5mL/100µL/5.00mL/MSVOA_N/MEOH
ALS Vial : 24 Sample Multiplier: 1

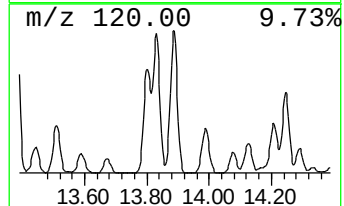
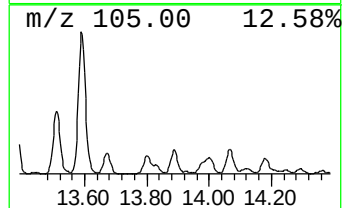
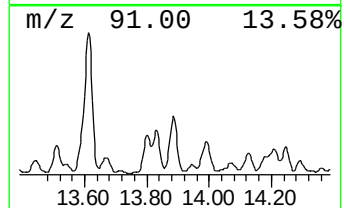
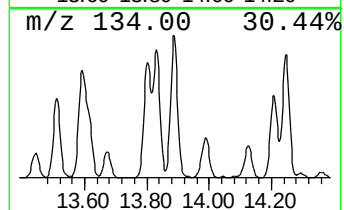
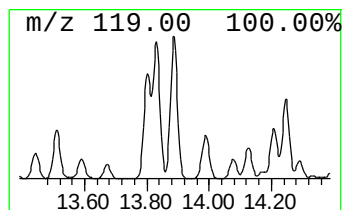
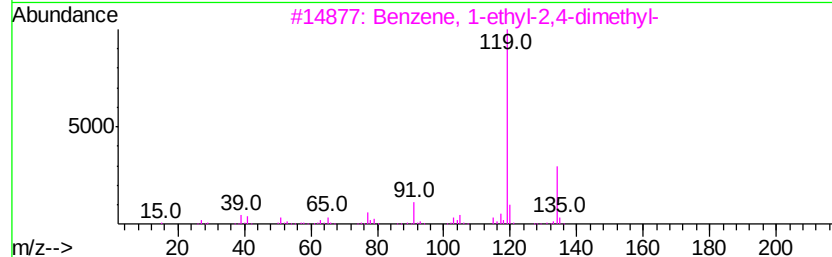
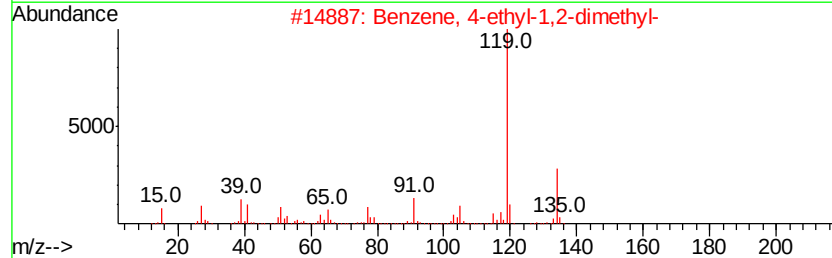
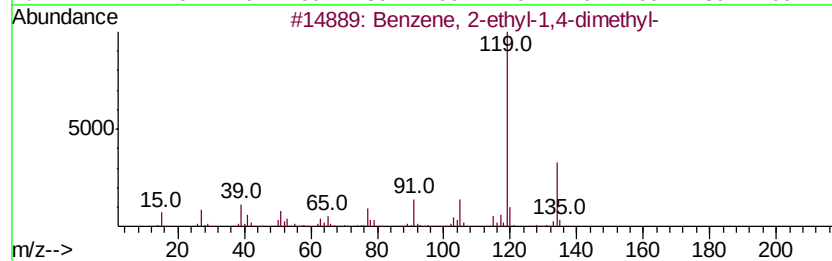
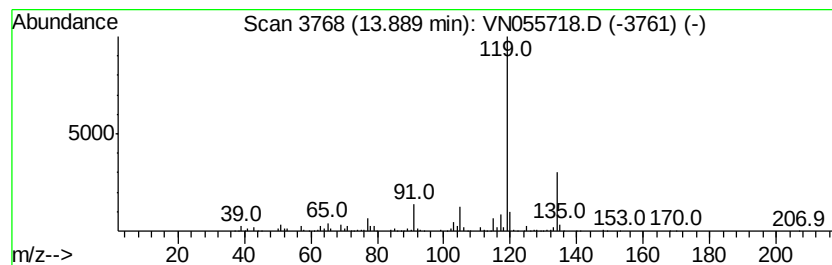
Instrument :
MSVOA_N
ClientSampleId :
EP1-W-2R(17-20)

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N051719W.M
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 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	92.16 ug/l	1042780	1,4-Dichlorobenzene-d4	13.34
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzene, 2-ethyl-1,4-dimethyl-	134 C10H14	001758-88-9 97
2		Benzene, 4-ethyl-1,2-dimethyl-	134 C10H14	000934-80-5 95
3		Benzene, 1-ethyl-2,4-dimethyl-	134 C10H14	000874-41-9 95
4		Benzene, 2-ethyl-1,3-dimethyl-	134 C10H14	002870-04-4 95
5		Benzene, 1-methyl-3-(1-methyleth...	134 C10H14	000535-77-3 94



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_N\DATA\VN052119\
Data File : VN055718.D
Acq On : 21 May 2019 18:43
Operator : JC/SP
Sample : K2977-04 50X
Misc : 5.61µ/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
EP1-W-2R(17-20)

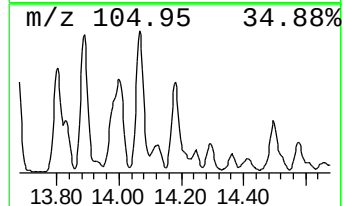
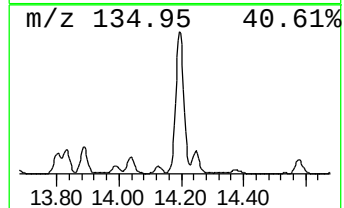
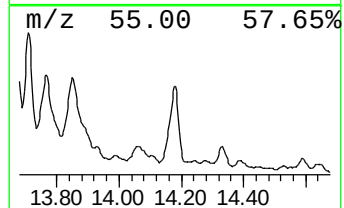
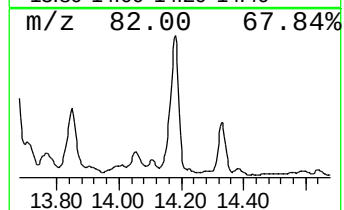
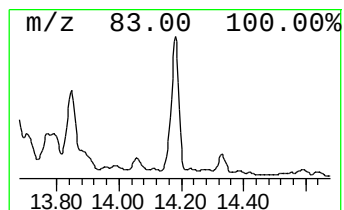
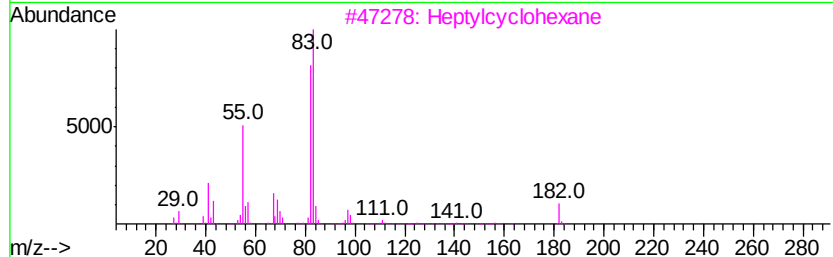
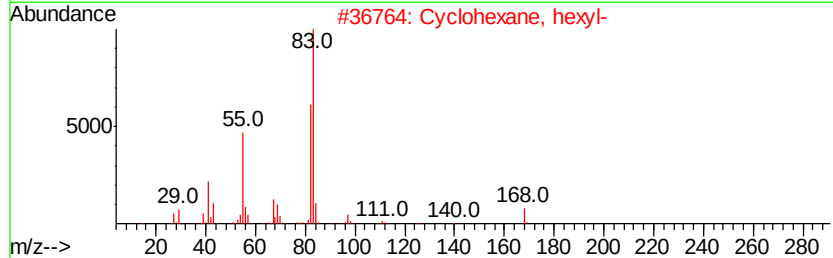
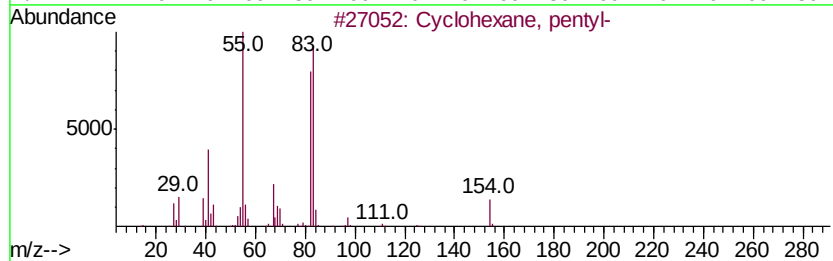
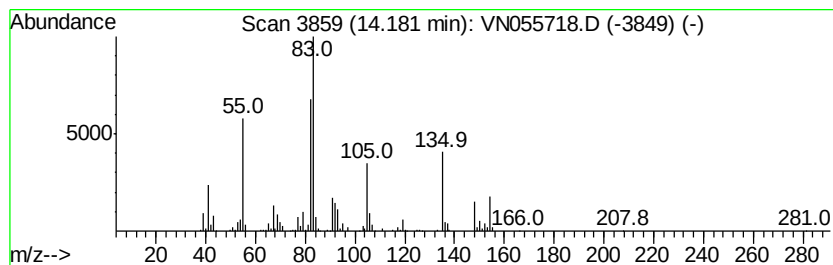
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N051719W.M
Quant Title : SW846 8260

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

Peak Number 10 unknown14.18 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.18	75.92 ug/l	859091	1,4-Dichlorobenzene-d4	13.34

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, pentyl-	154	C11H22	004292-92-6	49
2		Cyclohexane, hexyl-	168	C12H24	004292-75-5	43
3		Heptylcyclohexane	182	C13H26	005617-41-4	43
4		Cyclohexane, propyl-	126	C9H18	001678-92-8	43
5		n-Nonylcyclohexane	210	C15H30	002883-02-5	43



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN052119\
Data File : VN055718.D
Acq On : 21 May 2019 18:43
Operator : JC/SP
Sample : K2977-04 50X
Misc : 5.61g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
EP1-W-2R(17-20)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N051719W.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-et...	11.92	85.5	ug/l	2542680	3	11.41	1486810	50.0
Cyclohexane, propyl-	12.16	106.0	ug/l	3150680	3	11.41	1486810	50.0
unknown12.49	12.49	96.4	ug/l	1090410	4	13.34	565772	50.0
Cyclohexane, 1-me...	12.64	95.5	ug/l	1081140	4	13.34	565772	50.0
Cyclohexane, 1-me...	12.73	472.3	ug/l	5344280	4	13.34	565772	50.0
Sulfurous acid, d...	12.78	125.2	ug/l	1416320	4	13.34	565772	50.0
Nonane, 2,6-dimet...	12.96	292.4	ug/l	3308280	4	13.34	565772	50.0
Benzene, 1-methyl...	13.83	69.0	ug/l	780667	4	13.34	565772	50.0
Benzene, 2-ethyl-...	13.89	92.2	ug/l	1042780	4	13.34	565772	50.0
unknown14.18	14.18	75.9	ug/l	859091	4	13.34	565772	50.0