

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN051319\
 Data File : VN055573.D
 Acq On : 13 May 2019 12:28
 Operator : JC/SP
 Sample : K2704-01
 Misc : 5.47g/5mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 SB-2(24.5)

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\82N050819W.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	2.551	206	242	243	rBV3	107046	377832	8.63%	0.641%
2	7.590	1787	1809	1820	rBV2	507904	1287681	29.40%	2.186%
3	7.664	1820	1832	1877	rVB	897873	2246879	51.31%	3.815%
4	8.024	1925	1944	1966	rBV	616302	1422928	32.49%	2.416%
5	8.583	2103	2118	2166	rVB	1353695	3022105	69.01%	5.131%
6	9.078	2247	2272	2284	rBV3	80002	197288	4.51%	0.335%
7	9.725	2461	2473	2496	rVB3	50294	130104	2.97%	0.221%
8	9.866	2497	2517	2537	rVB6	30255	92791	2.12%	0.158%
9	10.088	2569	2586	2620	rBV	2146781	4379297	100.00%	7.435%
10	10.255	2632	2638	2657	rVB	44487	128660	2.94%	0.218%
11	10.432	2685	2693	2709	rVB3	54489	107781	2.46%	0.183%
12	10.525	2709	2722	2734	rBV6	48263	114113	2.61%	0.194%
13	10.622	2745	2752	2761	rVB6	27427	46003	1.05%	0.078%
14	10.715	2772	2781	2791	rVB2	88621	144794	3.31%	0.246%
15	10.818	2805	2813	2824	rVB3	29777	51840	1.18%	0.088%
16	10.882	2825	2833	2838	rBV5	30982	47704	1.09%	0.081%
17	10.950	2847	2854	2861	rVB	87831	126245	2.88%	0.214%
18	11.001	2861	2870	2882	rVB2	299581	533968	12.19%	0.907%
19	11.120	2896	2907	2916	rBV6	95701	182544	4.17%	0.310%
20	11.201	2916	2932	2953	rVB7	135201	414125	9.46%	0.703%
21	11.297	2953	2962	2982	rBV	188671	372072	8.50%	0.632%
22	11.406	2983	2996	3018	rBV	1855294	3443378	78.63%	5.846%
23	11.541	3032	3038	3044	rVB4	52603	68084	1.55%	0.116%
24	11.596	3044	3055	3063	rBV6	140975	288862	6.60%	0.490%
25	11.654	3065	3073	3081	rBV4	150892	297313	6.79%	0.505%
26	11.757	3096	3105	3112	rBV7	51843	92960	2.12%	0.158%
27	11.808	3114	3121	3128	rBV4	45313	69209	1.58%	0.117%
28	11.853	3129	3135	3142	rBV5	35951	48829	1.11%	0.083%
29	11.921	3142	3156	3169	rBV6	256665	701440	16.02%	1.191%
30	12.043	3186	3194	3202	rBV	351564	482345	11.01%	0.819%
31	12.117	3209	3217	3223	rBV3	276702	485656	11.09%	0.824%
32	12.400	3294	3305	3316	rBV	1544091	2737425	62.51%	4.647%
33	12.557	3345	3354	3369	rVB3	768614	1407939	32.15%	2.390%
34	12.644	3371	3381	3391	rBV8	219023	512508	11.70%	0.870%

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35	12.728	3393	3407	3416	rBV8	529276	1460361	33.35%	2.479%
36	12.863	3442	3449	3457	rBV7	246173	399148	9.11%	0.678%
37	12.959	3473	3479	3496	rVB6	583830	1095365	25.01%	1.860%
38	13.046	3500	3506	3512	rVV6	200438	271675	6.20%	0.461%
39	13.342	3589	3598	3616	rVB2	1733112	3295261	75.25%	5.594%
40	13.480	3634	3641	3648	rBV4	442413	670770	15.32%	1.139%
41	13.599	3670	3678	3686	rBV7	339502	720031	16.44%	1.222%
42	13.660	3688	3697	3707	rVB3	874788	1608293	36.72%	2.730%
43	13.995	3791	3801	3810	rBV3	1065542	1867618	42.65%	3.171%
44	14.172	3848	3856	3863	rBV4	715085	1347416	30.77%	2.287%
45	14.290	3887	3893	3899	rBV3	544490	790718	18.06%	1.342%
46	14.329	3900	3905	3912	rVB3	761798	1018772	23.26%	1.730%
47	14.522	3960	3965	3973	rVB2	746315	1001425	22.87%	1.700%
48	14.580	3974	3983	3996	rBV3	1522519	3228698	73.73%	5.481%
49	14.647	3997	4004	4013	rBV5	586936	1145219	26.15%	1.944%
50	14.850	4061	4067	4073	rBV3	780922	997046	22.77%	1.693%
51	14.956	4091	4100	4112	rVB3	1232496	2484524	56.73%	4.218%
52	15.239	4181	4188	4197	rBV5	795844	1732822	39.57%	2.942%
53	15.908	4386	4396	4408	rVB3	1163461	2251643	51.42%	3.823%
54	16.097	4448	4455	4465	rVB3	869557	1599295	36.52%	2.715%
55	16.162	4468	4475	4483	rBV4	577357	1096329	25.03%	1.861%
56	16.348	4522	4533	4545	rBV6	1144219	2758374	62.99%	4.683%

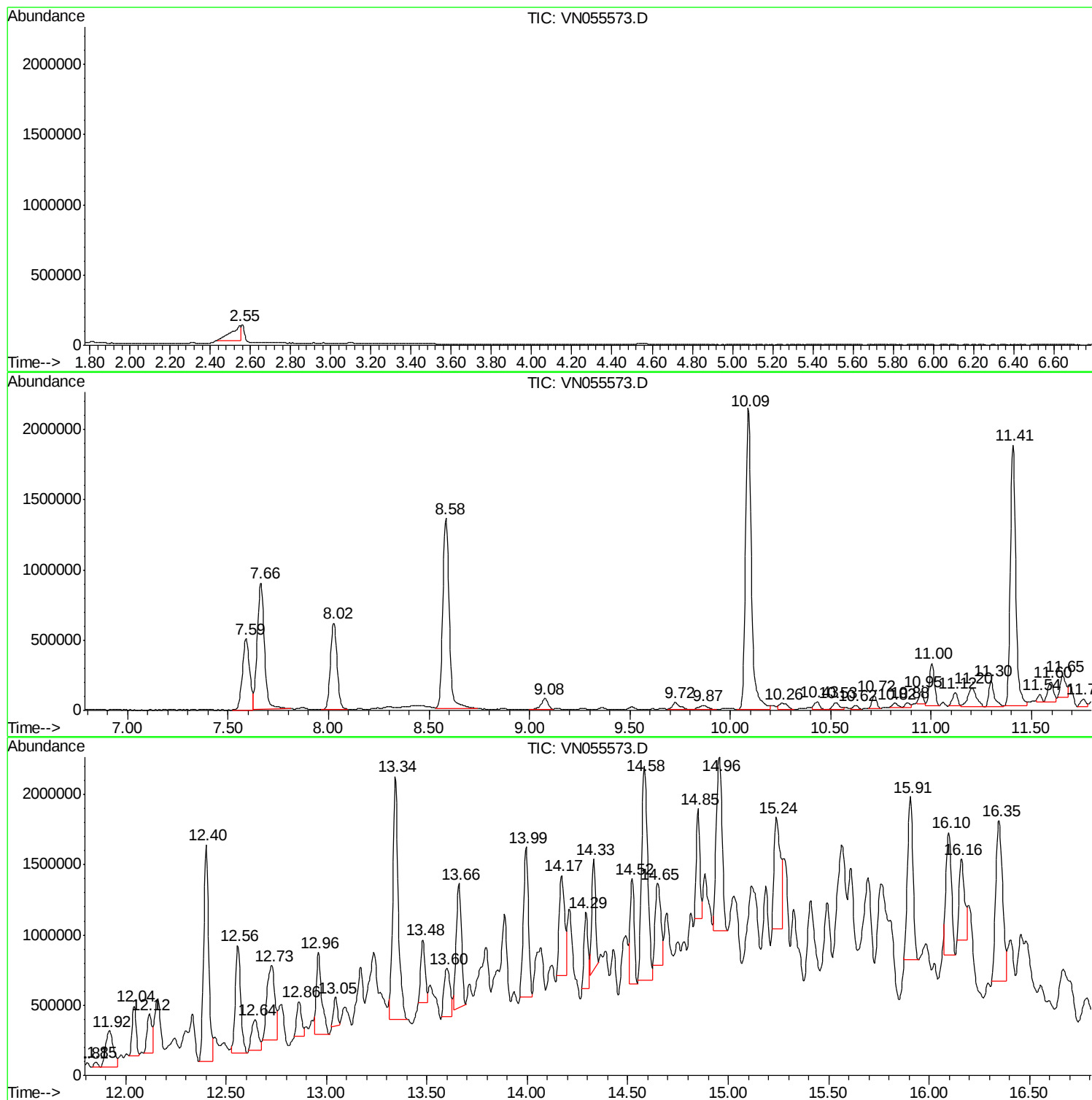
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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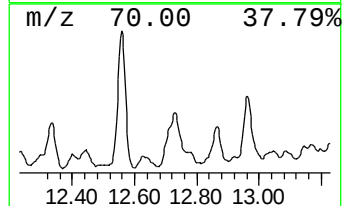
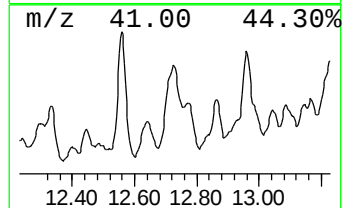
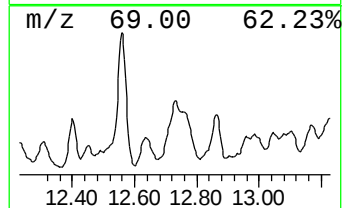
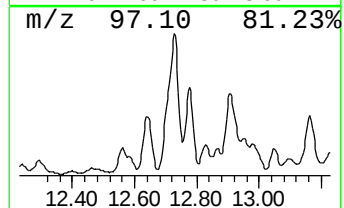
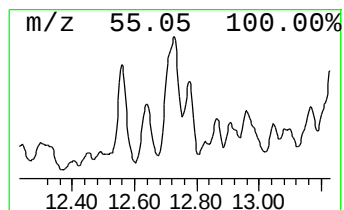
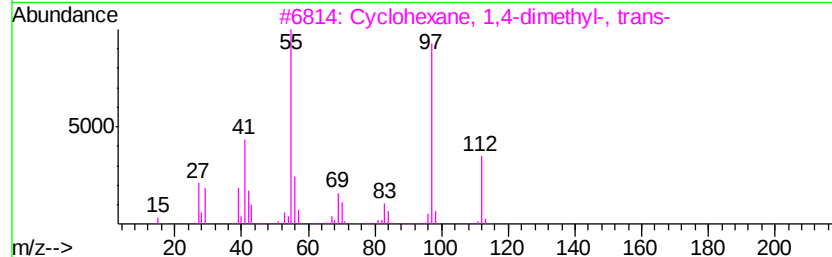
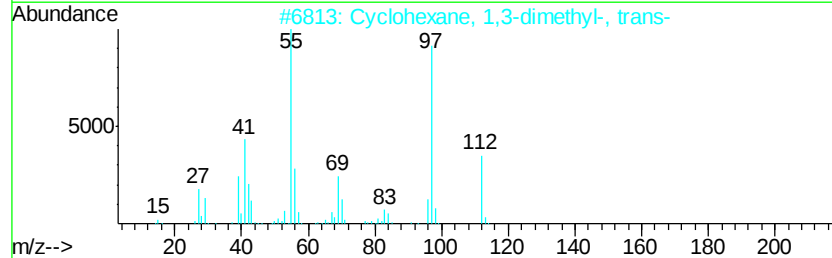
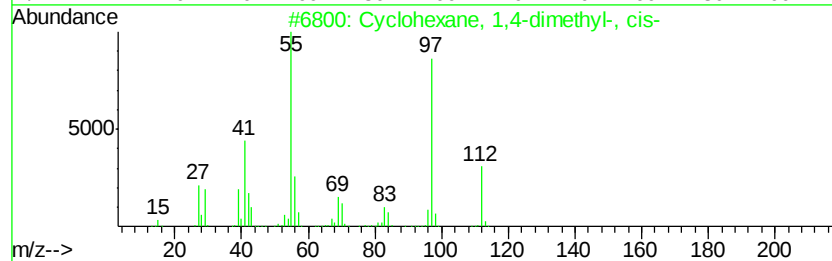
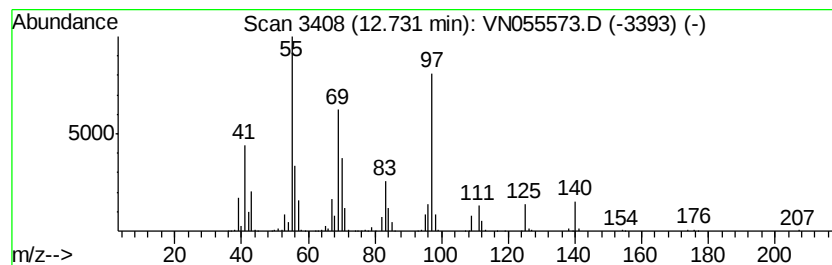
Instrument :
MSVOA_N
ClientSampleId :
SB-2(24.5)

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N050819W.M
Quant Title : SW846 8260

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

Peak Number 1 Cyclohexane, 1,4-dimethyl-,... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.73	22.16 ug/l	1460360	1,4-Dichlorobenzene-d4	13.34
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Cyclohexane, 1,4-dimethyl-, cis-	112 C8H16	000624-29-3 62
2		Cyclohexane, 1,3-dimethyl-, trans-	112 C8H16	002207-03-6 52
3		Cyclohexane, 1,4-dimethyl-, trans-	112 C8H16	002207-04-7 52
4		Cyclohexane, 1,1-dimethyl-	112 C8H16	000590-66-9 49
5		Cyclohexane, 1-methyl-3-propyl-	140 C10H20	004291-80-9 49



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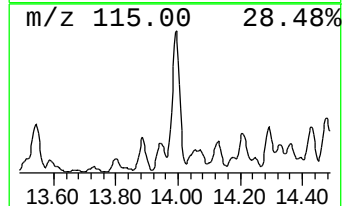
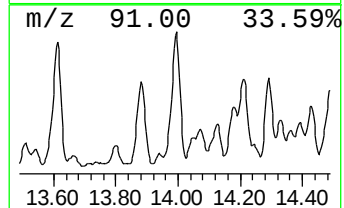
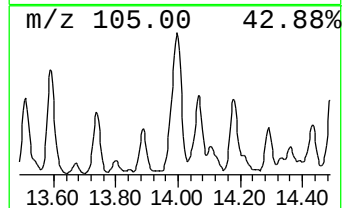
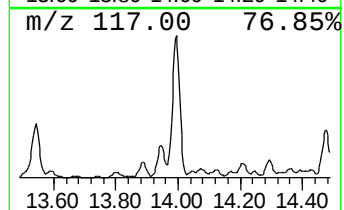
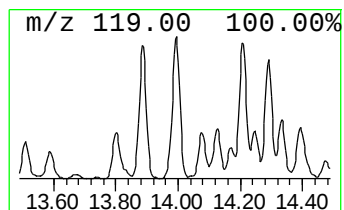
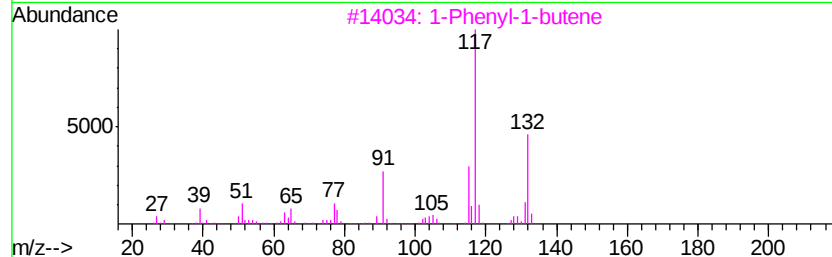
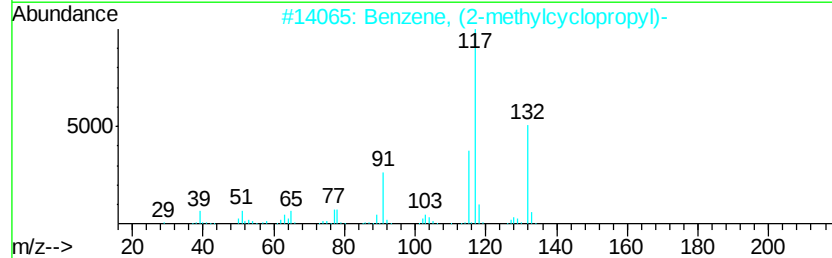
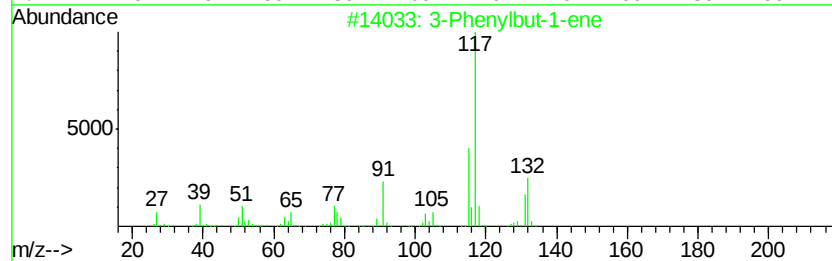
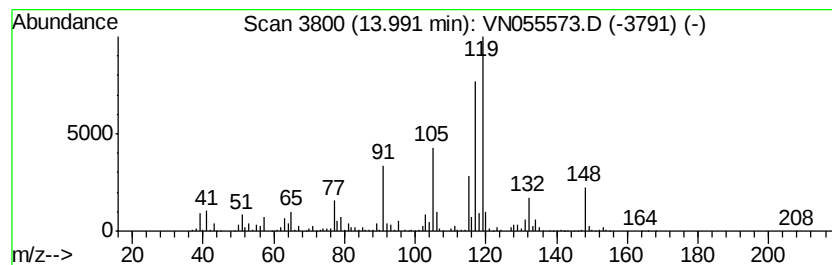
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown13.99 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.99	28.34 ug/l	1867620	1,4-Dichlorobenzene-d4	13.34

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Phenylbut-1-ene	132	C10H12	000934-10-1	46
2		Benzene, (2-methylcyclopropyl)-	132	C10H12	1000327-39-0	46
3		1-Phenyl-1-butene	132	C10H12	000824-90-8	46
4		Benzene, 2-butenyl-	132	C10H12	001560-06-1	42
5		Benzene, (2-methyl-2-propenyl)-	132	C10H12	003290-53-7	42



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ALS Vial : 9 Sample Multiplier: 1

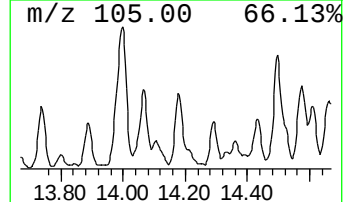
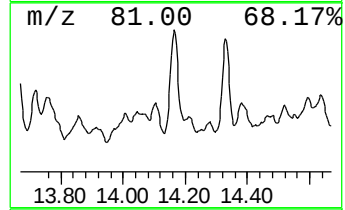
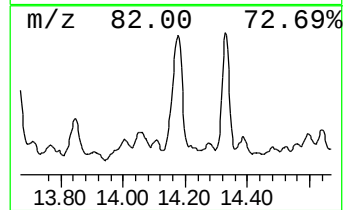
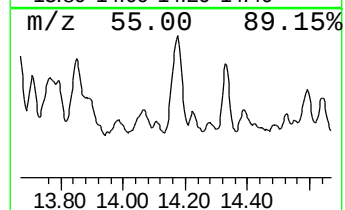
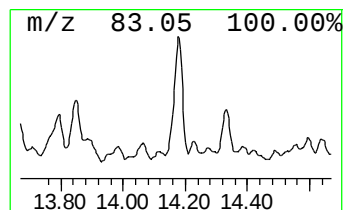
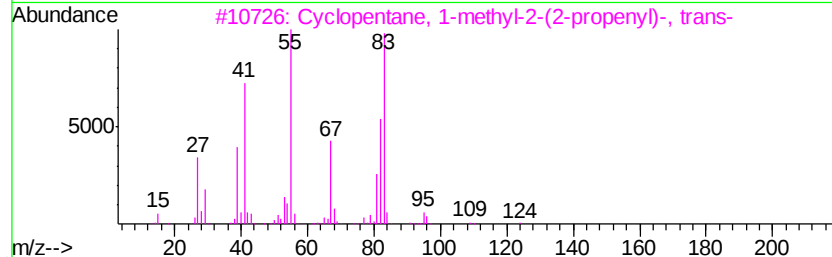
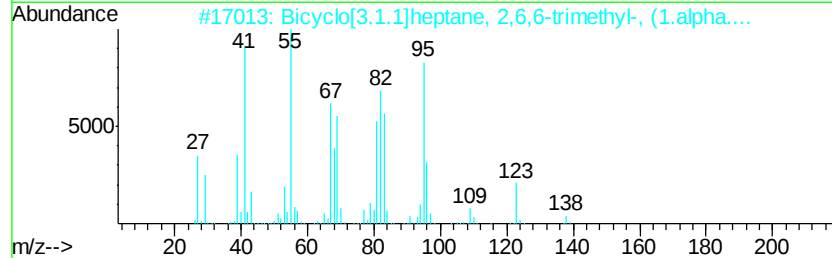
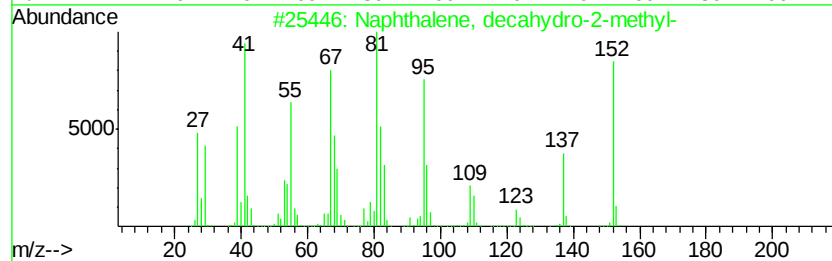
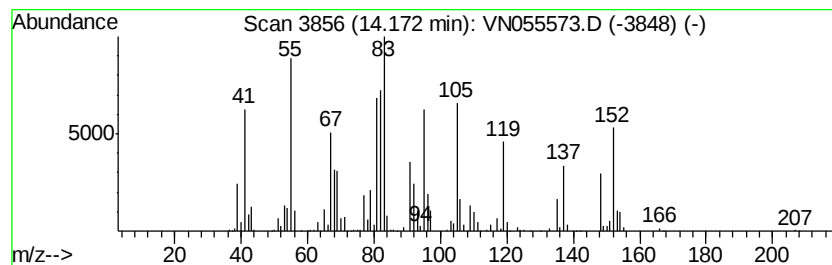
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 Naphthalene, decahydro-2-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.17	20.44 ug/l	1347420	1,4-Dichlorobenzene-d4	13.34
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Naphthalene, decahydro-2-methyl-	152 C11H20	002958-76-1 89
2		Bicyclo[3.1.1]heptane, 2,6,6-tri...	138 C10H18	006876-13-7 38
3		Cyclopentane, 1-methyl-2-(2-prop...	124 C9H16	050746-53-7 38
4		Bicyclo[4.1.0]heptan-3-one, 4,7,...	152 C10H16O	004176-01-6 27
5		Bicyclo[4.1.0]heptan-3-one, 4,7,...	152 C10H16O	004176-04-9 27



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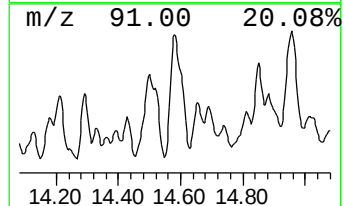
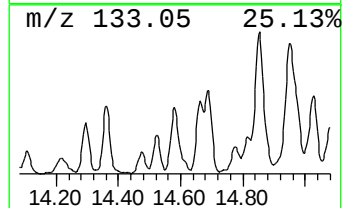
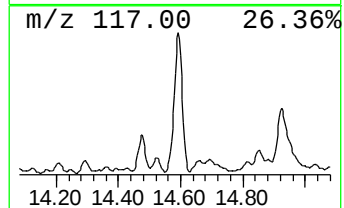
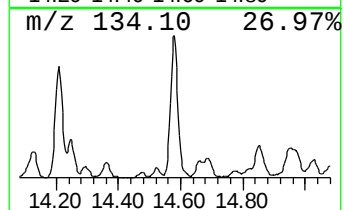
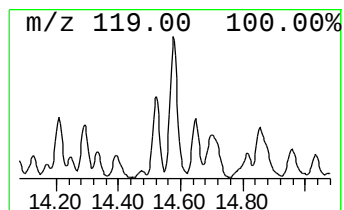
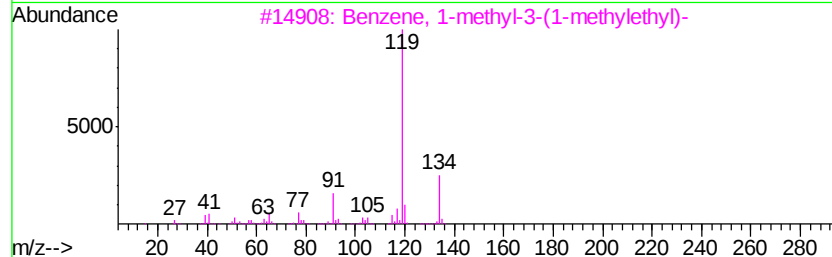
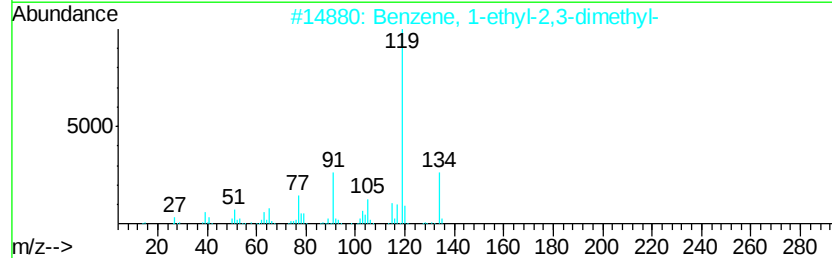
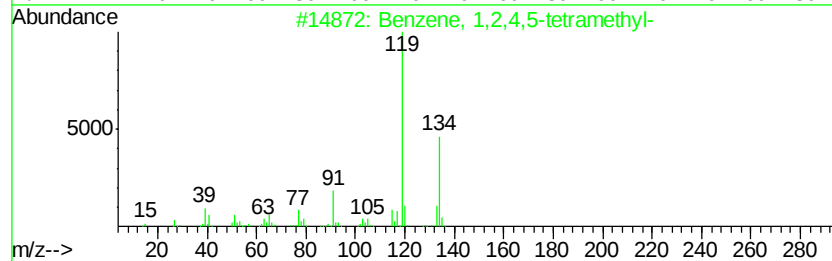
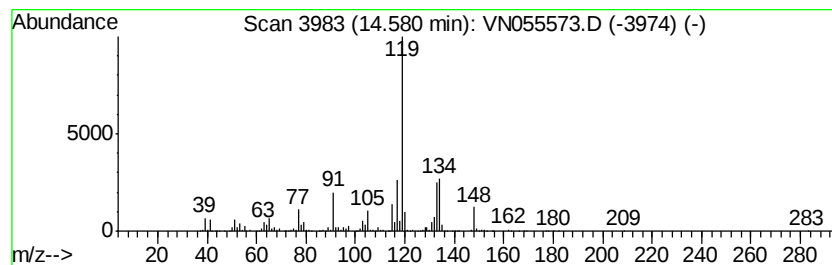
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.58	48.99 ug/l	3228700	1,4-Dichlorobenzene-d4	13.34

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	70
2		Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	64
3		Benzene, 1-methyl-3-(1-methylethyl)-	134	C10H14	000535-77-3	64
4		Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	64
5		o-Cymene	134	C10H14	000527-84-4	64



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ALS Vial : 9 Sample Multiplier: 1

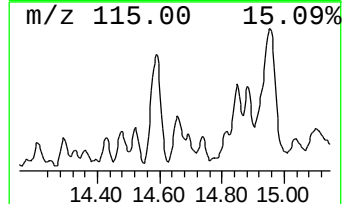
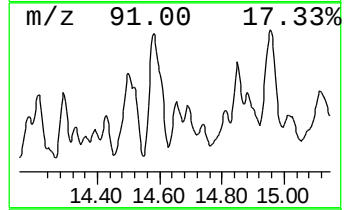
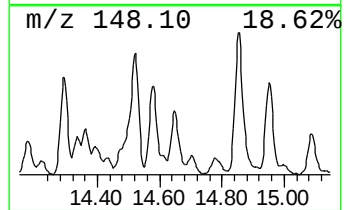
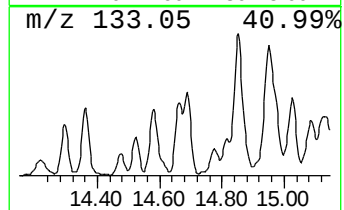
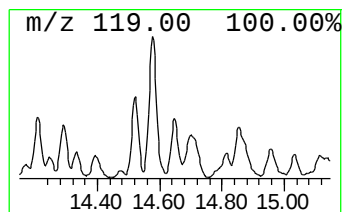
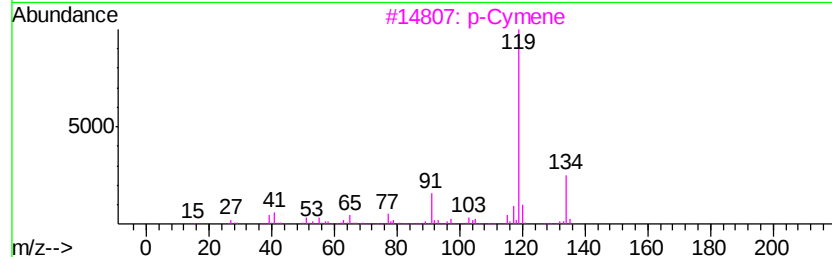
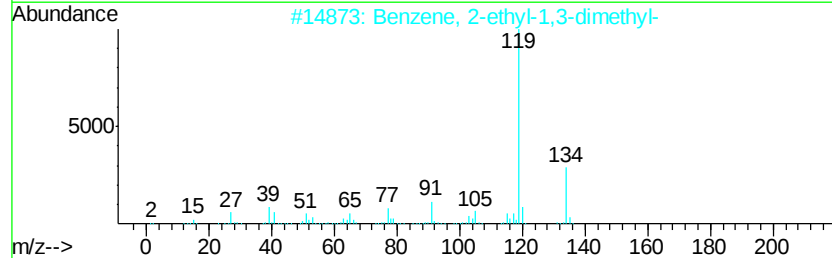
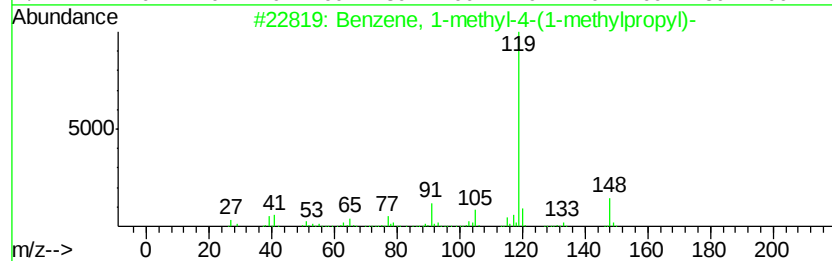
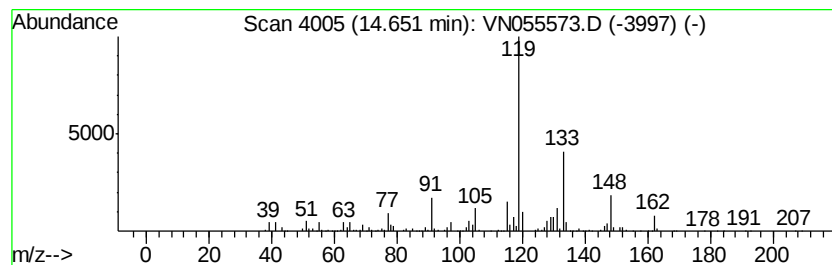
Instrument :
MSVOA_N
ClientSampleId :
SB-2(24.5)

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N050819W.M
Quant Title : SW846 8260

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

Peak Number 5 Benzene, 1-methyl-4-(1-meth... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.65	17.38 ug/l	1145220	1,4-Dichlorobenzene-d4	13.34
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzene, 1-methyl-4-(1-methylpro...	148 C11H16	001595-16-0 64
2		Benzene, 2-ethyl-1,3-dimethyl-	134 C10H14	002870-04-4 60
3		p-Cymene	134 C10H14	000099-87-6 53
4		Benzene, 1,2,3,4-tetramethyl-	134 C10H14	000488-23-3 50
5		Propiophenone, 2'-methyl-	148 C10H12O	002040-14-4 50



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA N\DATA\VN051319\
Data File : VN055573.D
Acq On : 13 May 2019 12:28
Operator : JC/SP
Sample : K2704-01
Misc : 5.47uL/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SB-2(24.5)

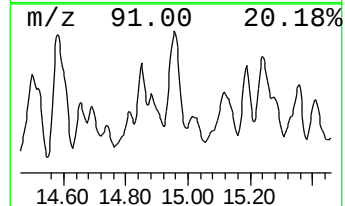
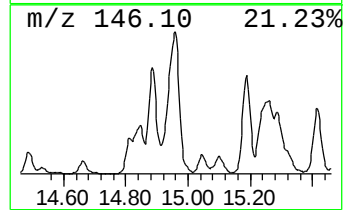
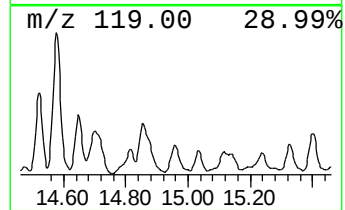
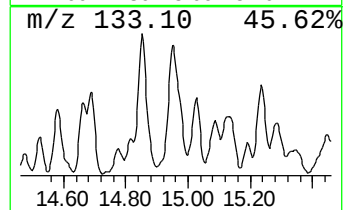
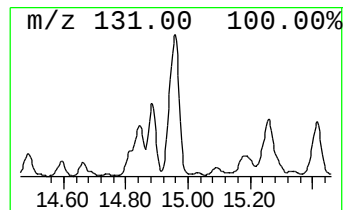
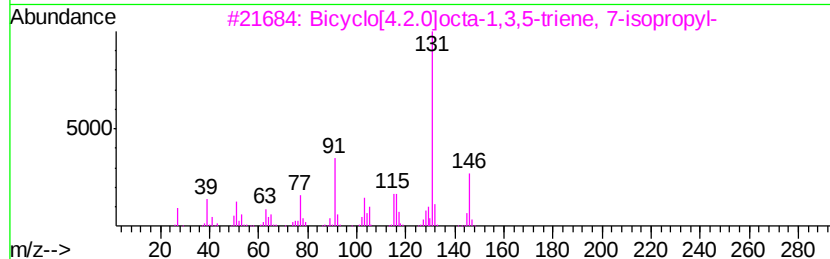
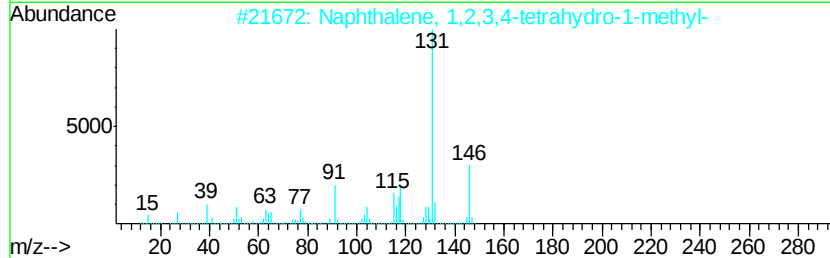
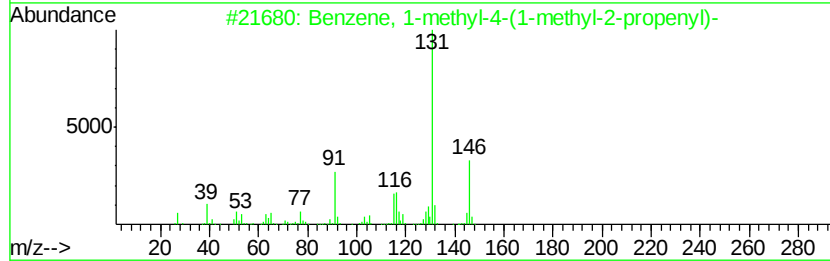
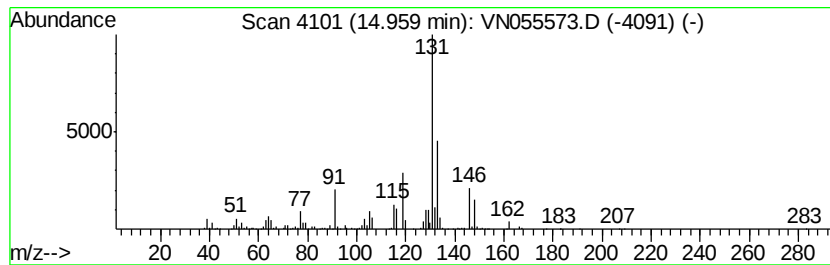
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Quant Title : SW846 8260

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

Peak Number 6 Benzene, 1-methyl-4-(1-meth... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.96	37.70 ug/l	2484520	1,4-Dichlorobenzene-d4	13.34

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-methyl-4-(1-methyl-2-...	146	C11H14	097664-18-1	64
2		Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001559-81-5	64
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	146	C11H14	027087-54-3	64
4		2,2-Dimethylindene, 2,3-dihydro-	146	C11H14	020836-11-7	64
5		1H-Indene, 2,3-dihydro-1,3-dimet...	146	C11H14	004175-53-5	64



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA N\DATA\VN051319\
Data File : VN055573.D
Acq On : 13 May 2019 12:28
Operator : JC/SP
Sample : K2704-01
Misc : 5.47uL/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SB-2(24.5)

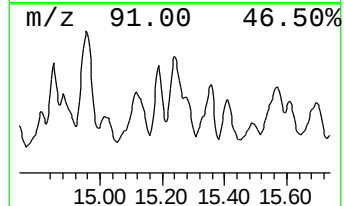
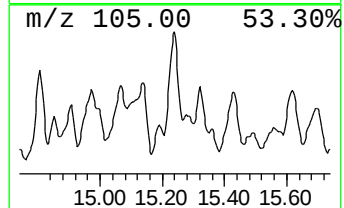
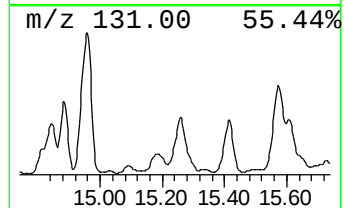
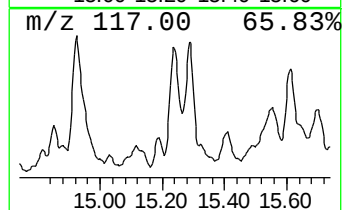
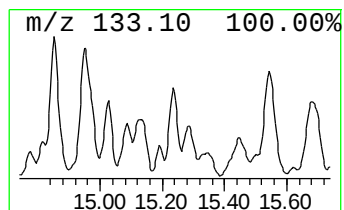
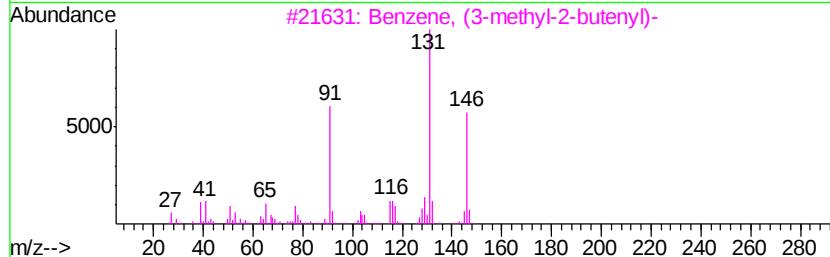
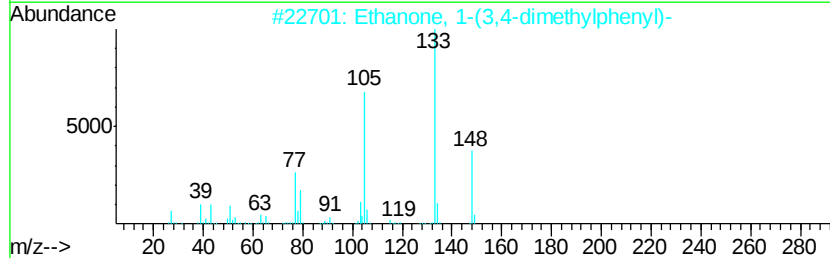
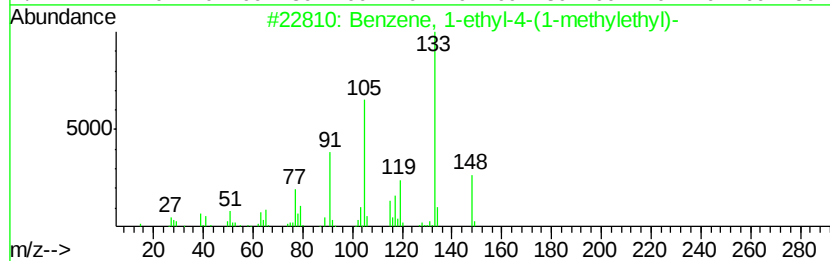
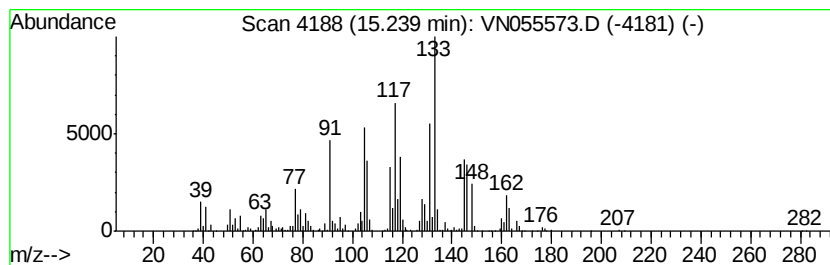
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Quant Title : SW846 8260

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

Peak Number 7 unknown15.24 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.24	26.29 ug/l	1732820	1,4-Dichlorobenzene-d4	13.34

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-ethyl-4-(1-methylethyl)-	148	C11H16	004218-48-8	46
2		Ethanone, 1-(3,4-dimethylphenyl)-	148	C10H12O	003637-01-2	25
3		Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	25
4		1-Propanone, 1-(2,4-dimethylphenyl)-	162	C11H14O	035031-55-1	20
5		Naphthalene, 1,2,3,4-tetrahydro-	146	C11H14	001680-51-9	20



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA N\DATA\VN051319\
Data File : VN055573.D
Acq On : 13 May 2019 12:28
Operator : JC/SP
Sample : K2704-01
Misc : 5.47uL/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

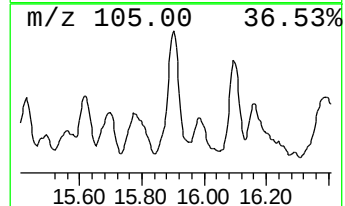
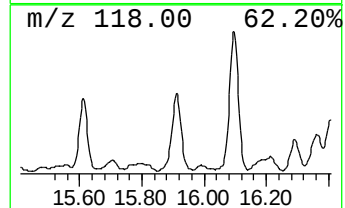
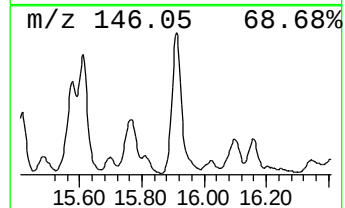
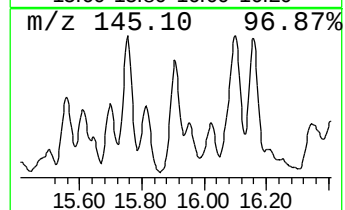
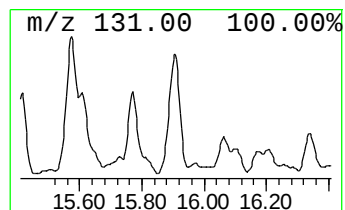
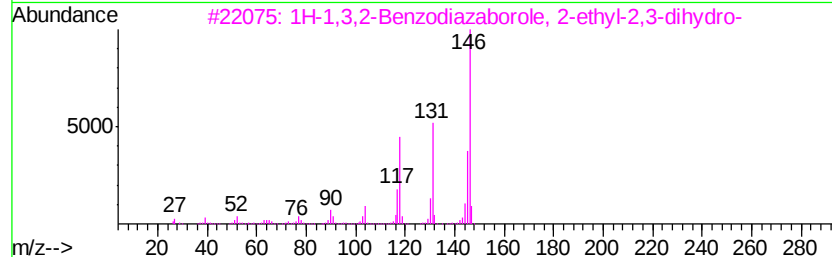
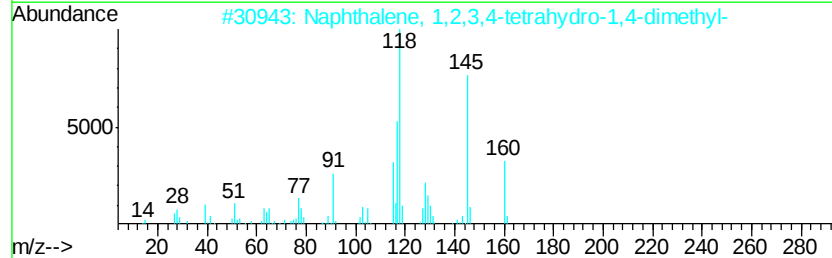
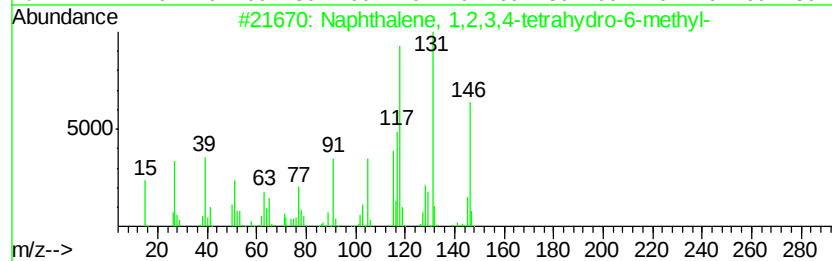
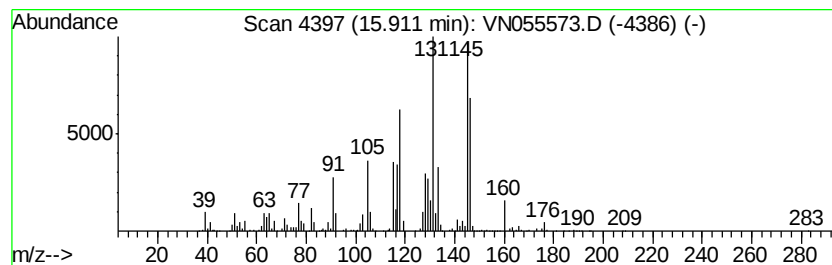
Instrument :
MSVOA_N
ClientSampleId :
SB-2(24.5)

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N050819W.M
Quant Title : SW846 8260

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

Peak Number 8 Naphthalene, 1,2,3,4-tetra... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.91	34.16 ug/l	2251640	1,4-Dichlorobenzene-d4	13.34
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Naphthalene, 1,2,3,4-tetrahydro-...	146 C11H14	001680-51-9 60
2		Naphthalene, 1,2,3,4-tetrahydro-...	160 C12H16	004175-54-6 55
3		1H-1,3,2-Benzodiazaborole, 2-eth...	146 C8H11BN2	074663-81-3 53
4		Naphthalene, 1,2,3,4-tetrahydro-...	146 C11H14	002809-64-5 53
5		1H-Benzimidazole, 2-ethyl-	146 C9H10N2	001848-84-6 52



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA N\DATA\VN051319\
Data File : VN055573.D
Acq On : 13 May 2019 12:28
Operator : JC/SP
Sample : K2704-01
Misc : 5.47µ/5mL/100µL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SB-2(24.5)

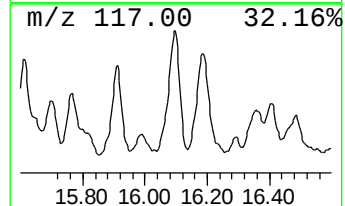
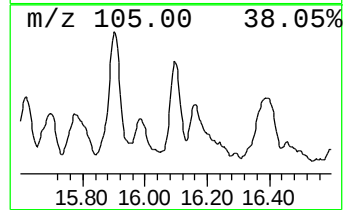
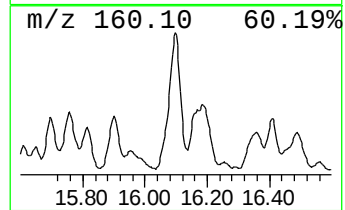
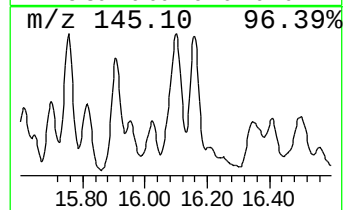
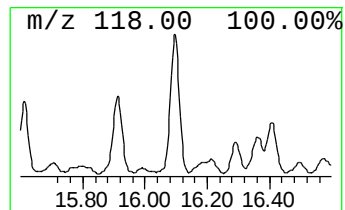
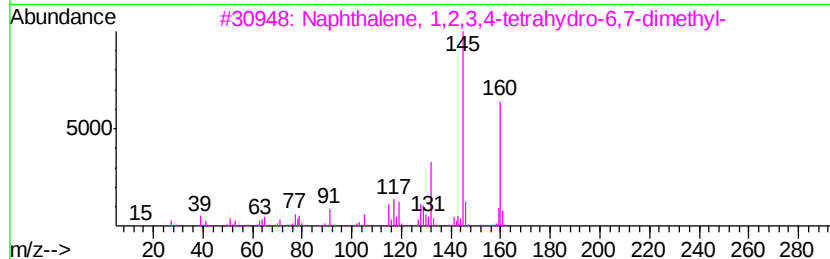
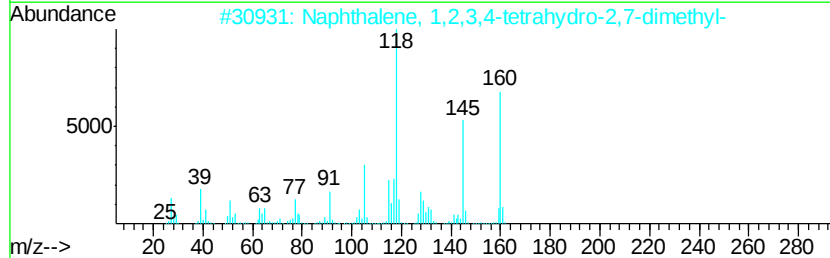
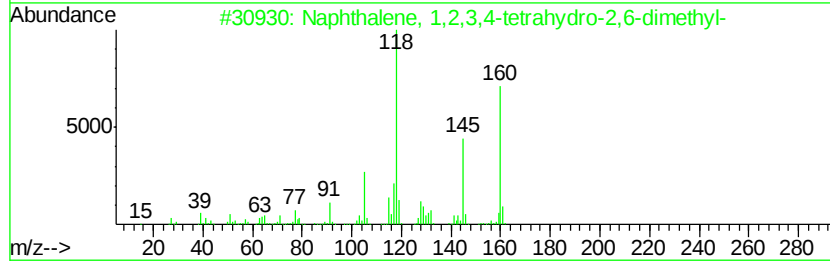
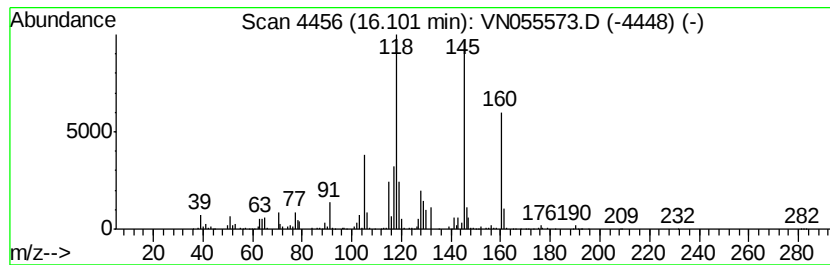
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Quant Title : SW846 8260

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

Peak Number 9 Naphthalene, 1,2,3,4-tetra... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.10	24.27 ug/l	1599300	1,4-Dichlorobenzene-d4	13.34

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	007524-63-2	76
2		Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	013065-07-1	76
3		Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	001076-61-5	60
4		Benzene, 1-(1-methylethenyl)-3-(...	160	C12H16	001129-29-9	60
5		Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	020027-77-4	60



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA N\DATA\VN051319\
Data File : VN055573.D
Acq On : 13 May 2019 12:28
Operator : JC/SP
Sample : K2704-01
Misc : 5.47µL/100µL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

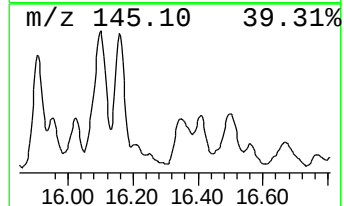
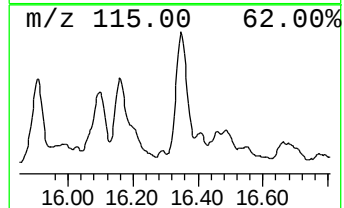
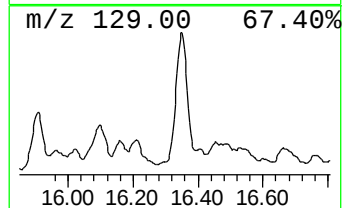
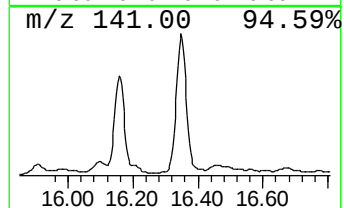
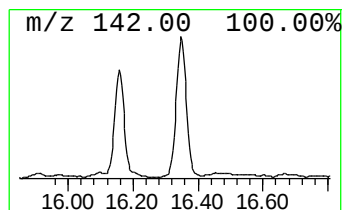
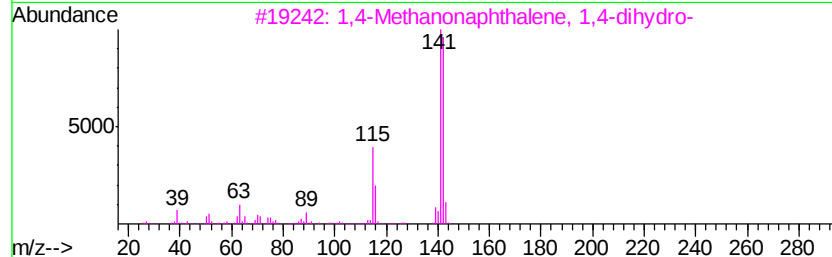
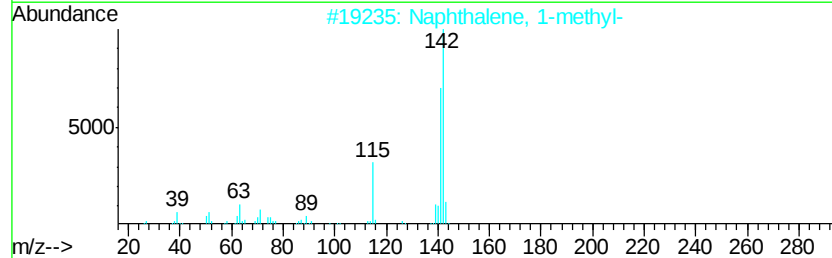
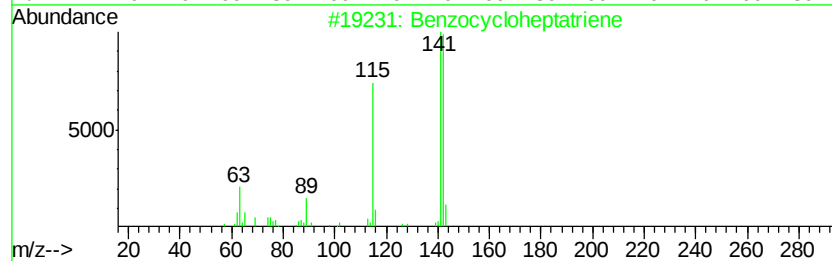
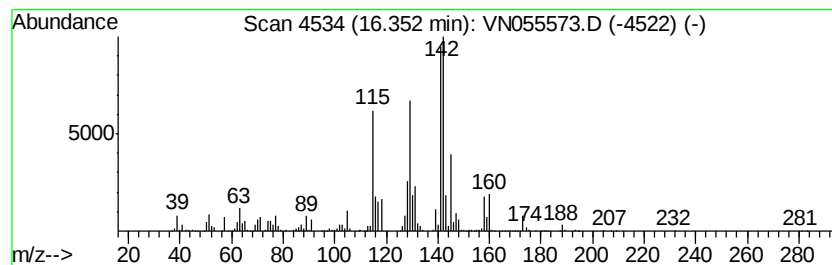
Instrument :
MSVOA_N
ClientSampled :
SB-2(24.5)

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N050819W.M
Quant Title : SW846 8260

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

Peak Number 10 Benzocycloheptatriene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.35	41.85 ug/l	2758370	1,4-Dichlorobenzene-d4	13.34
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzocycloheptatriene	142 C11H10	000264-09-5 55
2		Naphthalene, 1-methyl-	142 C11H10	000090-12-0 50
3		1,4-Methanonaphthalene, 1,4-dihydro-	142 C11H10	004453-90-1 50
4		Naphthalene, 2-methyl-	142 C11H10	000091-57-6 50
5		Spiro(tricyclo[6.2.1.0(2,7)]undec-5-en-2-ylidene)-	186 C13H14O	1000210-02-3 50



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN051319\
Data File : VN055573.D
Acq On : 13 May 2019 12:28
Operator : JC/SP
Sample : K2704-01
Misc : 5.47g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SB-2(24.5)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N050819W.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, 1,4-...	12.73	22.2	ug/l	1460360	4	13.34	3295260	50.0
unknown13.99	13.99	28.3	ug/l	1867620	4	13.34	3295260	50.0
Naphthalene, deca...	14.17	20.4	ug/l	1347420	4	13.34	3295260	50.0
Benzene, 1,2,4,5-...	14.58	49.0	ug/l	3228700	4	13.34	3295260	50.0
Benzene, 1-methyl...	14.65	17.4	ug/l	1145220	4	13.34	3295260	50.0
Benzene, 1-methyl...	14.96	37.7	ug/l	2484520	4	13.34	3295260	50.0
unknown15.24	15.24	26.3	ug/l	1732820	4	13.34	3295260	50.0
Naphthalene, 1,2,...	15.91	34.2	ug/l	2251640	4	13.34	3295260	50.0
Naphthalene, 1,2,...	16.10	24.3	ug/l	1599300	4	13.34	3295260	50.0
Benzocycloheptatr...	16.35	41.9	ug/l	2758370	4	13.34	3295260	50.0