

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN062119\
 Data File : VN056427.D
 Acq On : 21 Jun 2019 15:39
 Operator : JC/SP
 Sample : K3482-05
 Misc : 5.19g/5mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 TP-3

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\82N061919W.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	1787	1809	1820	rBV2	186831	482466	3.72%	0.231%
2	7.660	1820	1831	1846	rVB	332187	767520	5.92%	0.368%
3	7.870	1881	1896	1928	rVB2	65979	174276	1.35%	0.084%
4	8.024	1928	1944	1968	rBV	211829	490790	3.79%	0.235%
5	8.583	2102	2118	2159	rVB	561492	1182552	9.13%	0.567%
6	9.043	2246	2261	2268	rBV	123192	265314	2.05%	0.127%
7	9.085	2270	2274	2282	rVV	110092	176232	1.36%	0.084%
8	9.140	2282	2291	2304	rVB2	160932	319819	2.47%	0.153%
9	9.361	2339	2360	2379	rBV2	270637	635708	4.91%	0.305%
10	9.506	2391	2405	2426	rVB3	411581	843642	6.51%	0.404%
11	9.664	2432	2454	2461	rBV	234684	472549	3.65%	0.227%
12	9.757	2474	2483	2496	rVB	540570	964794	7.45%	0.462%
13	9.863	2497	2516	2522	rBV6	368243	1090194	8.41%	0.523%
14	9.976	2540	2551	2571	rBV5	127887	402406	3.11%	0.193%
15	10.085	2571	2585	2611	rBV3	2123648	4306676	33.24%	2.064%
16	10.213	2613	2625	2630	rBV	263494	471718	3.64%	0.226%
17	10.258	2630	2639	2659	rVB7	579891	1772521	13.68%	0.850%
18	10.394	2660	2681	2685	rBV	539108	1037240	8.01%	0.497%
19	10.432	2686	2693	2708	rVB	1041951	1855567	14.32%	0.889%
20	10.529	2709	2723	2732	rBV4	598782	1394348	10.76%	0.668%
21	10.577	2734	2738	2745	rVV2	314196	461810	3.56%	0.221%
22	10.625	2745	2753	2762	rVV2	808805	1287652	9.94%	0.617%
23	10.715	2771	2781	2793	rVB	2680634	4436576	34.24%	2.127%
24	10.818	2800	2813	2826	rBV	1283343	2861718	22.09%	1.372%
25	10.885	2827	2834	2840	rBV4	581446	928429	7.17%	0.445%
26	11.004	2858	2871	2882	rBV	6125490	11747324	90.67%	5.631%
27	11.059	2883	2888	2894	rVV3	629123	912211	7.04%	0.437%
28	11.117	2895	2906	2915	rVV5	2368273	4922604	37.99%	2.360%
29	11.197	2915	2931	2951	rVB5	2554453	8866309	68.43%	4.250%
30	11.297	2951	2962	2972	rBV	2888513	5204206	40.17%	2.495%
31	11.406	2987	2996	3003	rBV	819937	1415735	10.93%	0.679%
32	11.541	3030	3038	3044	rBV	1280494	2000043	15.44%	0.959%
33	11.590	3044	3053	3063	rVB6	2256395	4510658	34.81%	2.162%
34	11.654	3064	3073	3080	rBV	3311207	6096646	47.05%	2.922%

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Integration Parameters: RTEINT.P

Integrator: RTE
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Min Area: 3 % of largest Peak
Max Peaks: 100
Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
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35	11.757	3096	3105	3113	rBV3	1001454	1827159	14.10%	0.876%
36	11.853	3128	3135	3142	rVB5	780120	1119406	8.64%	0.537%
37	11.921	3143	3156	3169	rBV6	4289951	10387680	80.17%	4.979%
38	12.043	3187	3194	3202	rVB	4540085	5964168	46.03%	2.859%
39	12.120	3210	3218	3223	rBV2	3538728	5888818	45.45%	2.823%
40	12.159	3224	3230	3242	rVB4	5329185	9971931	76.96%	4.780%
41	12.336	3280	3285	3296	rVB3	3858069	5873647	45.33%	2.815%
42	12.403	3296	3306	3315	rBV7	1589400	3231400	24.94%	1.549%
43	12.561	3347	3355	3368	rVB3	6634018	11929847	92.08%	5.718%
44	12.641	3369	3380	3390	rBV7	2424758	5910857	45.62%	2.833%
45	12.725	3393	3406	3416	rBV5	4814845	12956661	100.00%	6.211%
46	12.866	3443	3450	3457	rVB5	2015053	2902696	22.40%	1.391%
47	12.924	3458	3468	3471	rVV2	1092511	2199950	16.98%	1.055%
48	12.959	3473	3479	3494	rVB2	4924771	8713500	67.25%	4.177%
49	13.596	3671	3677	3686	rBV8	752779	1504254	11.61%	0.721%
50	13.660	3688	3697	3707	rVV5	4564149	8580729	66.23%	4.113%
51	13.885	3762	3767	3777	rVB	3002793	4468512	34.49%	2.142%
52	13.991	3791	3800	3810	rVB8	1216323	2532619	19.55%	1.214%
53	14.171	3847	3856	3865	rBV7	2575012	5565786	42.96%	2.668%
54	14.290	3886	3893	3898	rBV3	1331391	1967860	15.19%	0.943%
55	14.329	3899	3905	3912	rVB2	1827718	2580642	19.92%	1.237%
56	14.580	3974	3983	3995	rVB2	4139341	7321836	56.51%	3.510%
57	14.644	3995	4003	4014	rBV4	1763379	2973501	22.95%	1.425%
58	14.956	4091	4100	4118	rVB3	2300658	4495458	34.70%	2.155%
59	15.236	4180	4187	4195	rBV3	766400	1342110	10.36%	0.643%
60	15.905	4386	4395	4407	rVB4	418776	839902	6.48%	0.403%
61	16.345	4522	4532	4557	rVB5	304500	811925	6.27%	0.389%

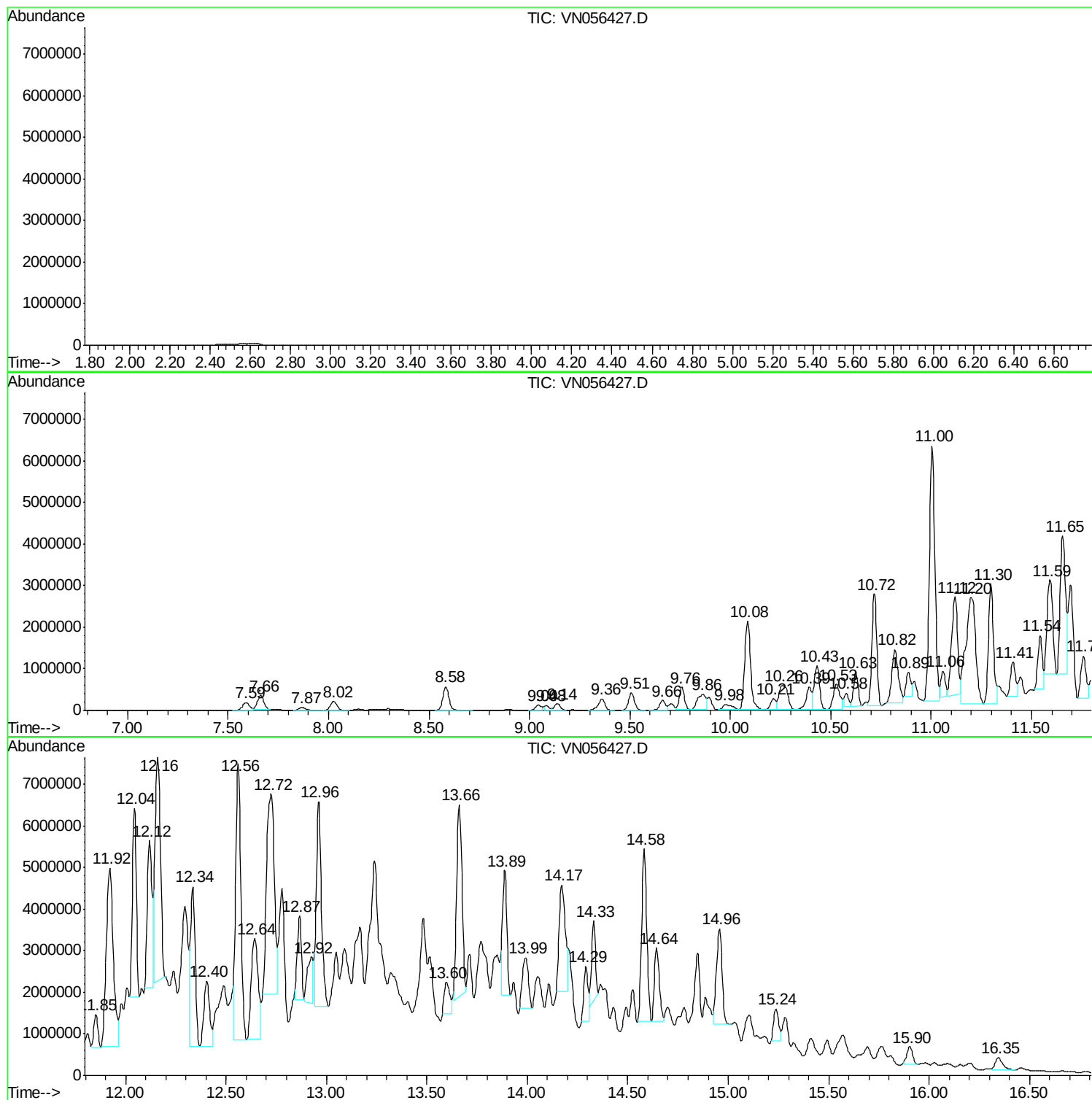
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N061919W.M
Quant Title : SW846 8260

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



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ALS Vial : 18 Sample Multiplier: 1

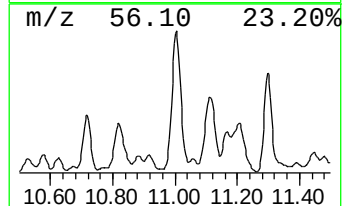
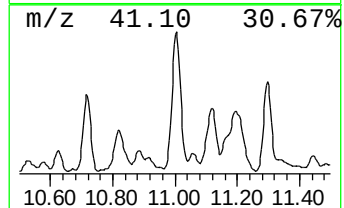
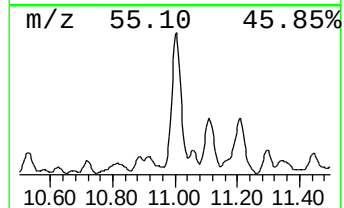
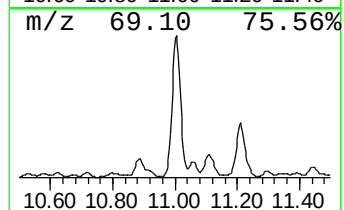
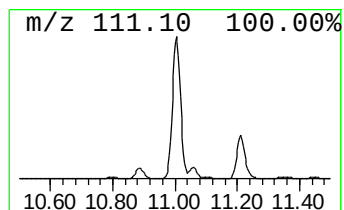
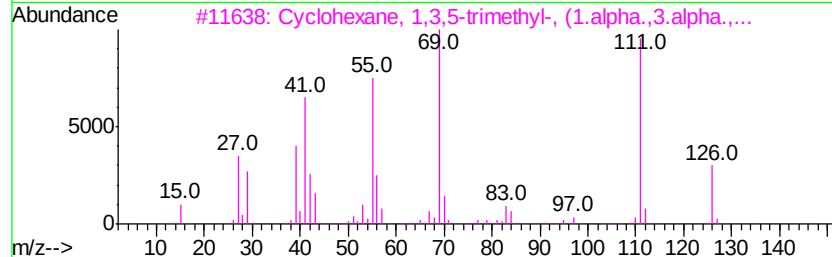
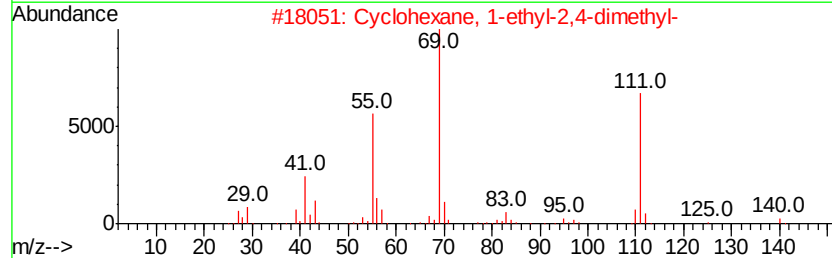
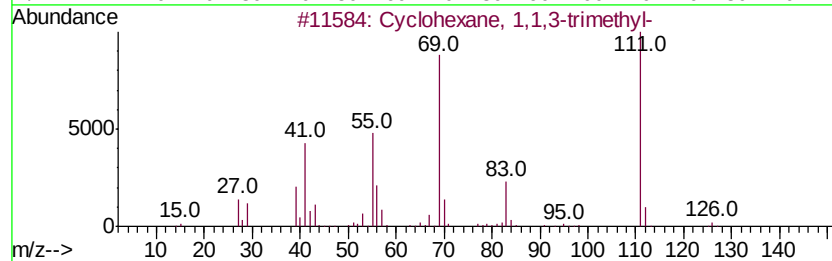
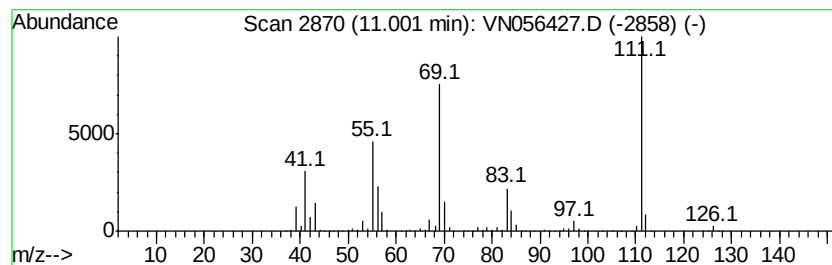
Instrument :
MSVOA_N
ClientSampled :
TP-3

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N061919W.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 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.00	414.88 ug/l	11747300	Chlorobenzene-d5	11.41	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,1,3-trimethyl-	126	C9H18	003073-66-3	94
2	Cyclohexane, 1-ethyl-2,4-dimethyl-	140	C10H20	061142-69-6	72
3	Cyclohexane, 1,3,5-trimethyl-, (...)	126	C9H18	001795-26-2	64
4	Cyclooctane, (1-methylpropyl)-	168	C12H24	016538-89-9	64
5	Cyclohexane, 1,2,4-trimethyl-	126	C9H18	002234-75-5	60



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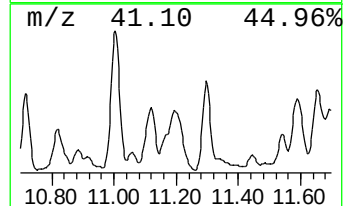
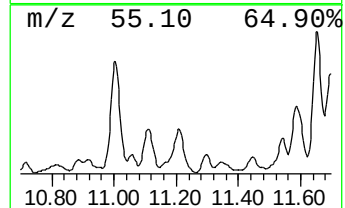
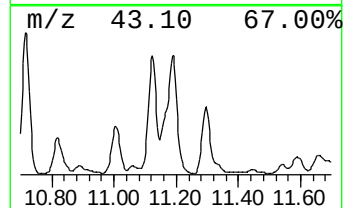
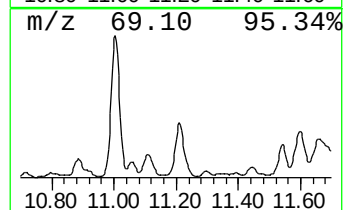
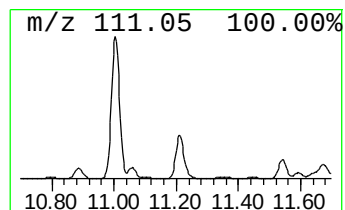
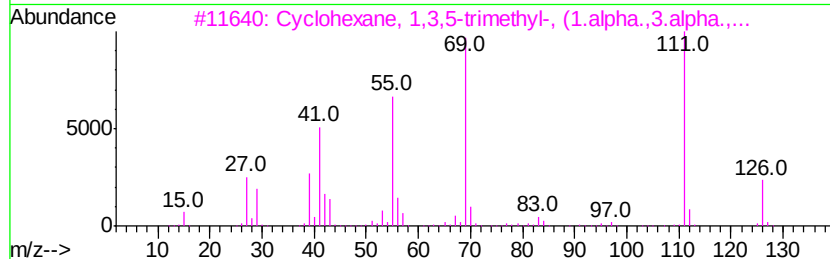
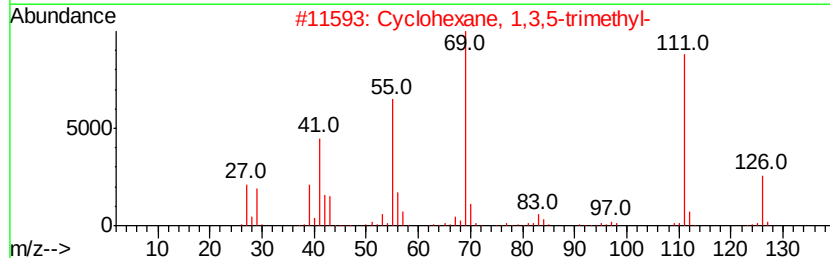
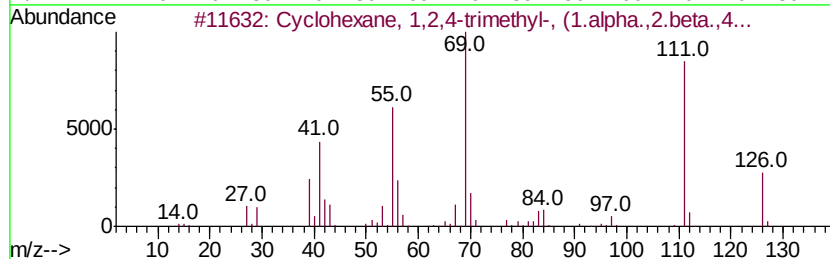
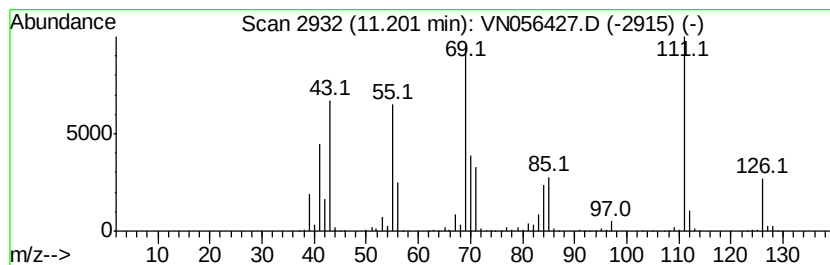
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Quant Title : SW846 8260

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

Peak Number 2 Cyclohexane, 1,2,4-trimethyl-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.		
11.20	313.13 ug/l	8866310	Chlorobenzene-d5	11.41		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclohexane, 1,2,4-trimethyl-, (...	126	C9H18	007667-60-9	60
2		Cyclohexane, 1,3,5-trimethyl-	126	C9H18	001839-63-0	46
3		Cyclohexane, 1,3,5-trimethyl-, (...	126	C9H18	001795-27-3	46
4		Cyclohexane, 1,2,4-trimethyl-	126	C9H18	002234-75-5	45
5		Cyclohexane, 1,2,3-trimethyl-, (...	126	C9H18	001839-88-9	43



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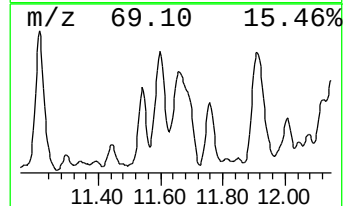
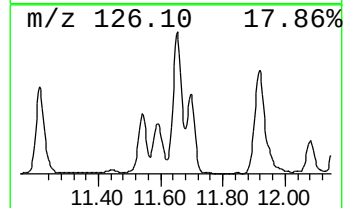
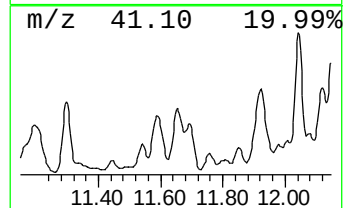
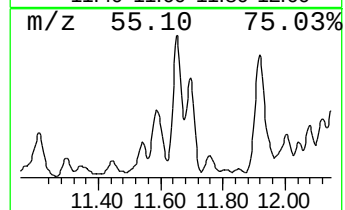
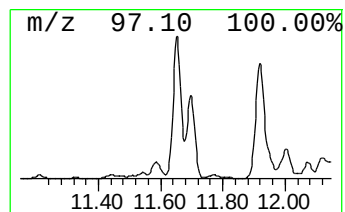
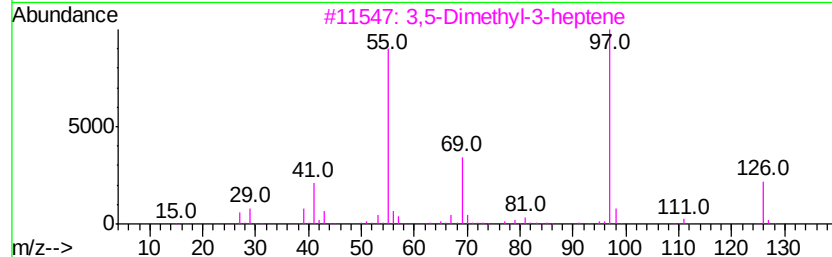
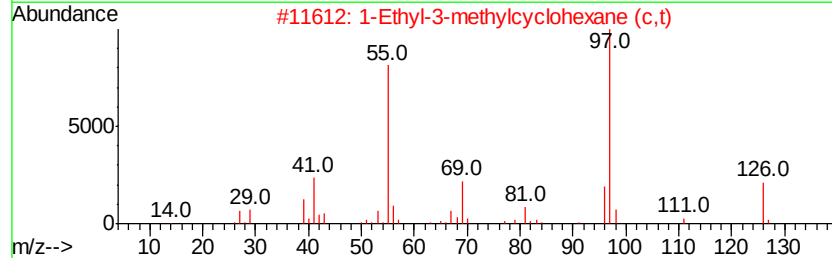
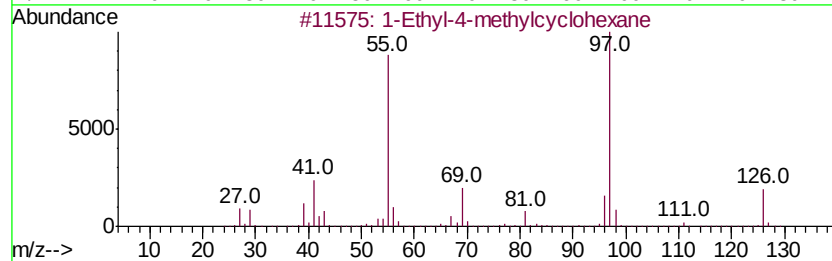
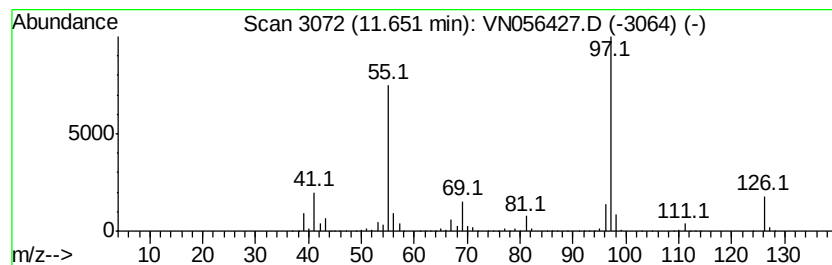
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Quant Title : SW846 8260

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

Peak Number 3 1-Ethyl-4-methylcyclohexane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.		
11.65	215.32 ug/l	6096650	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		3,5-Dimethyl-3-heptene	126	C9H18	059643-68-4	87
4		Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	004926-78-7	78
5		Sulfurous acid, cyclohexylmethyl...	346	C19H38O3S	1000309-22-0	72



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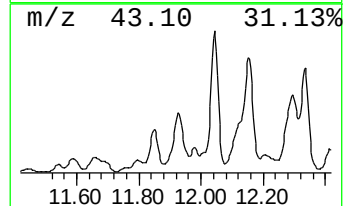
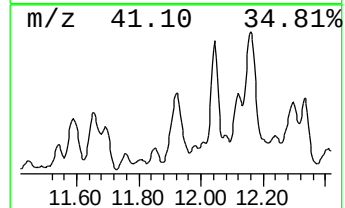
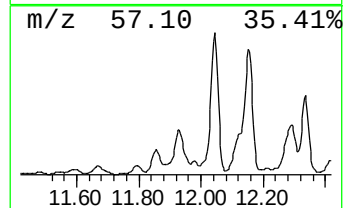
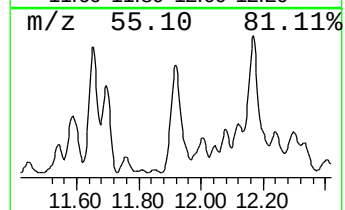
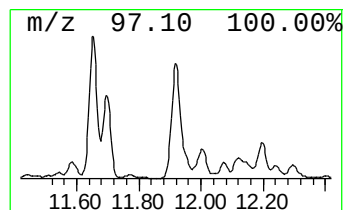
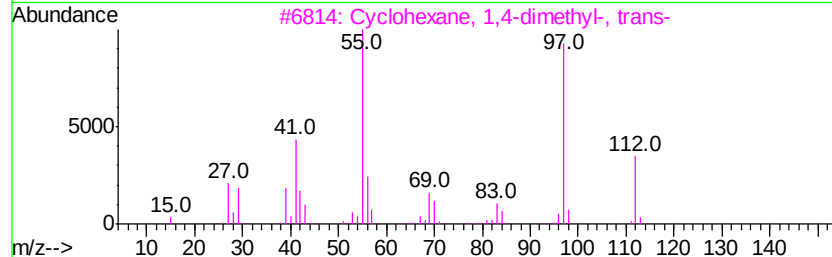
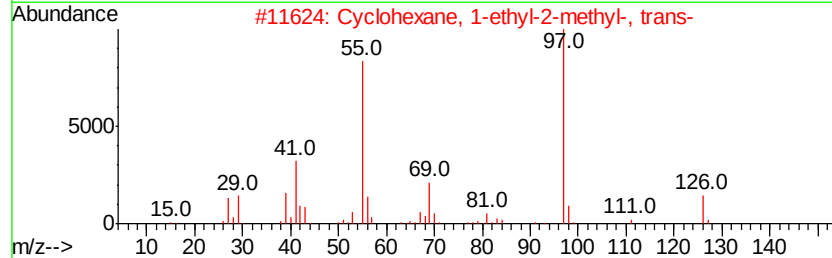
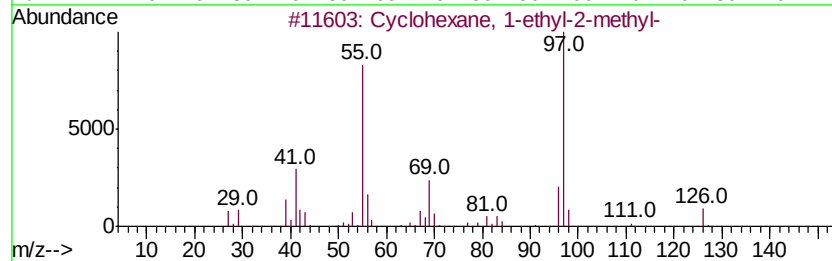
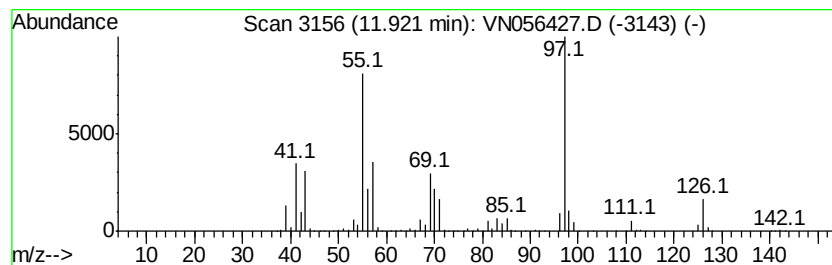
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Quant Title : SW846 8260

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

Peak Number 4 Cyclohexane, 1-ethyl-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	366.87 ug/l	10387700	Chlorobenzene-d5	11.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, 1-ethyl-2-methyl-	126	C9H18	003728-54-9	72
2		Cyclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-78-8	64
3		Cyclohexane, 1,4-dimethyl-, trans-	112	C8H16	002207-04-7	64
4		Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	59
5		3,5-Dimethyl-3-heptene	126	C9H18	059643-68-4	58



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Acq On : 21 Jun 2019 15:39
Operator : JC/SP
Sample : K3482-05
Misc : 5.19µ/5mL/100µL/5.00mL/MSVOA_N/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampled :
TP-3

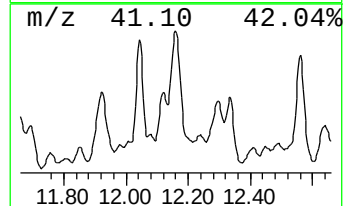
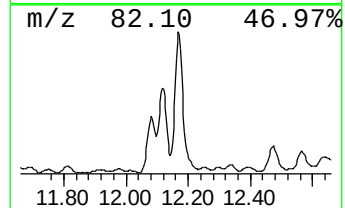
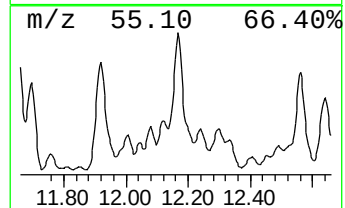
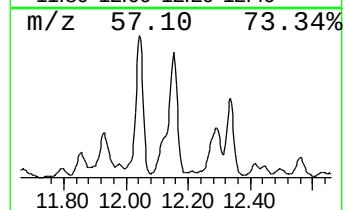
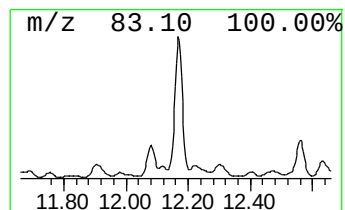
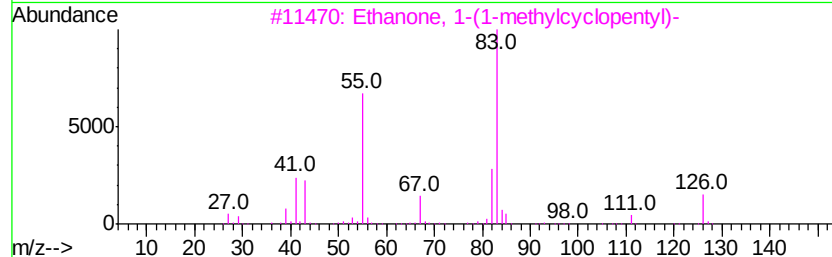
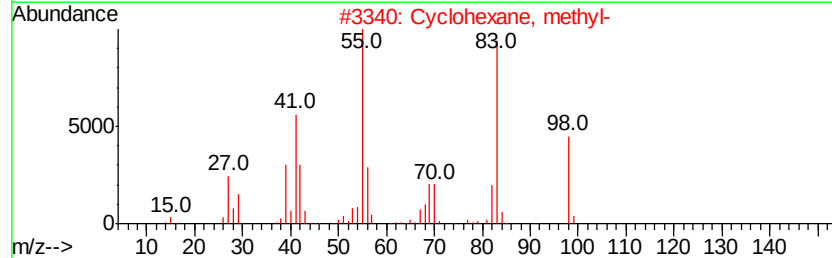
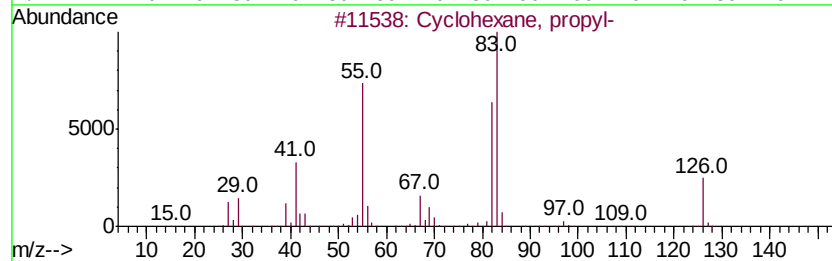
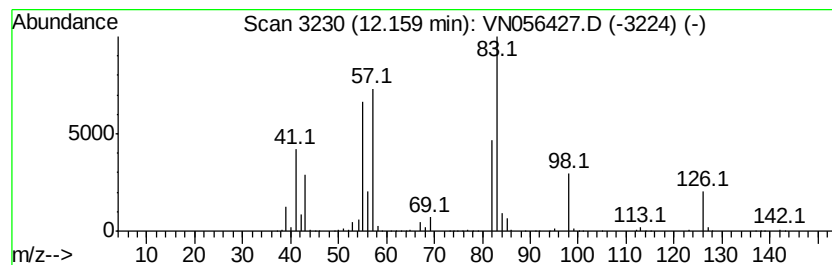
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Quant Title : SW846 8260

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

Peak Number 5 Cyclohexane, propyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.16	352.18 ug/l	9971930	Chlorobenzene-d5	11.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, propyl-	126	C9H18	001678-92-8	70
2		Cyclohexane, methyl-	98	C7H14	000108-87-2	50
3		Ethanone, 1-(1-methylcyclopentyl)-	126	C8H14O	013388-93-7	50
4		1H-Pyrazole, 4,5-dihydro-5,5-dim...	98	C5H10N2	004320-85-8	49
5		2-Pyrazoline, 1-methyl-4-propyl-	126	C7H14N2	033063-77-3	49



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA N\DATA\VN062119\
Data File : VN056427.D
Acq On : 21 Jun 2019 15:39
Operator : JC/SP
Sample : K3482-05
Misc : 5.19µ/5mL/100µL/5.00mL/MSVOA_N/MEOH
ALS Vial : 18 Sample Multiplier: 1

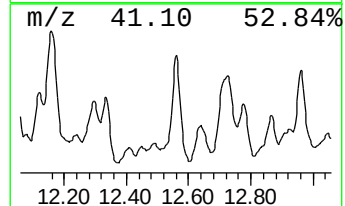
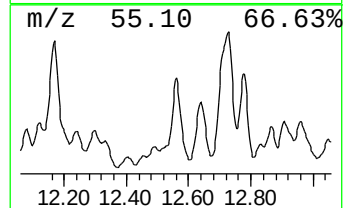
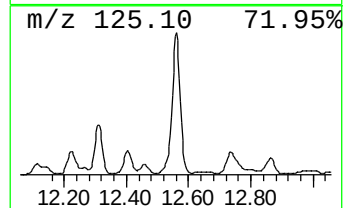
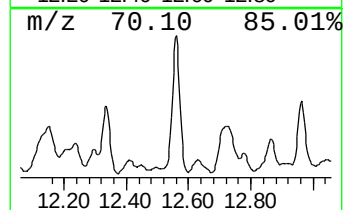
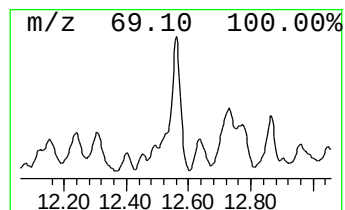
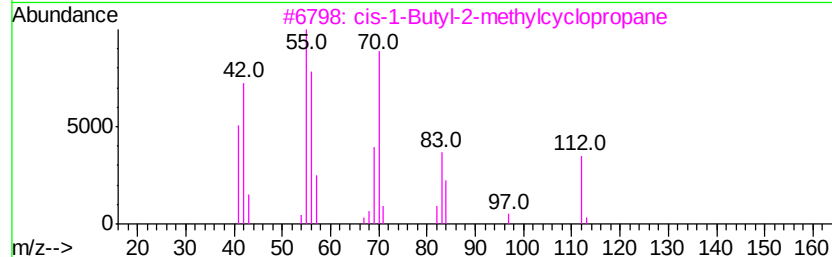
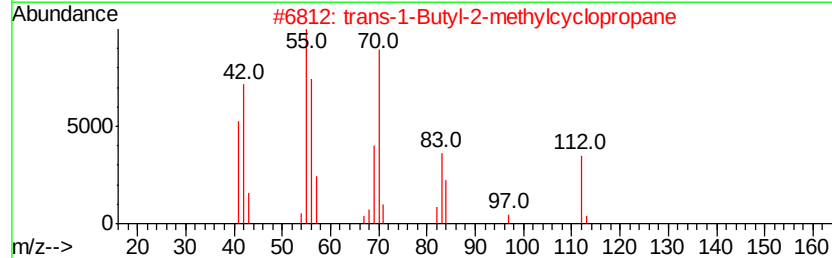
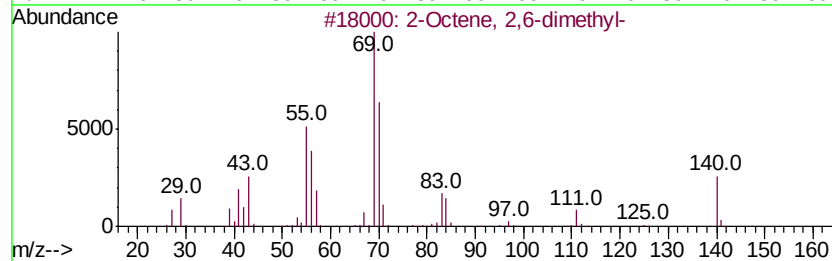
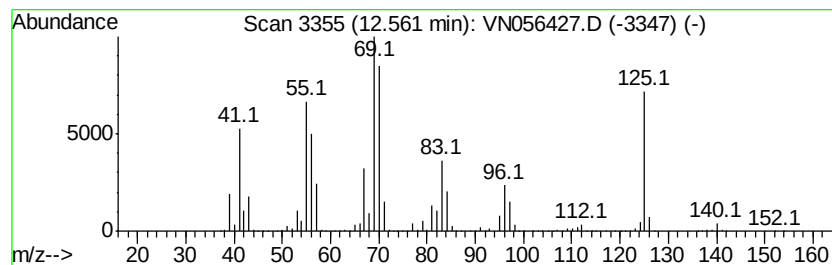
Instrument :
MSVOA_N
ClientSampled :
TP-3

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N061919W.M
Quant Title : SW846 8260

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

Peak Number 6 2-Octene, 2,6-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.56	396.54 ug/l	11929800	1,4-Dichlorobenzene-d4	13.34
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	2-Octene, 2,6-dimethyl-	140 C10H20	004057-42-5	58
2	trans-1-Butyl-2-methylcyclopropane	112 C8H16	038851-70-6	50
3	cis-1-Butyl-2-methylcyclopropane	112 C8H16	038851-69-3	50
4	Cyclopropane, 1,2-dimethyl-1-pen...	140 C10H20	062238-04-4	49
5	2-Ethylhexyl methacrylate	198 C12H22O2	000688-84-6	43



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_N\DATA\VN062119\
Data File : VN056427.D
Acq On : 21 Jun 2019 15:39
Operator : JC/SP
Sample : K3482-05
Misc : 5.19µL/100µL/5.00mL/MSVOA_N/MEOH
ALS Vial : 18 Sample Multiplier: 1

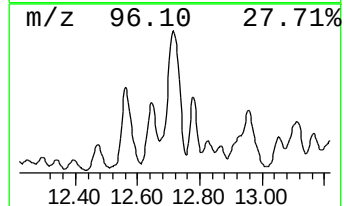
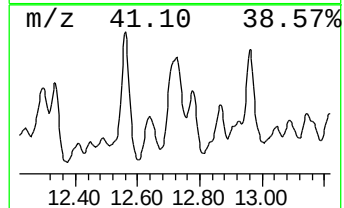
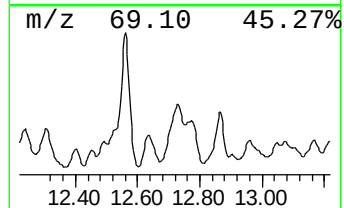
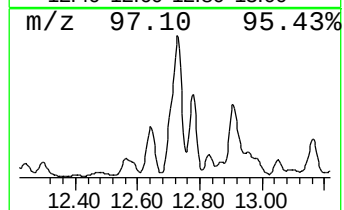
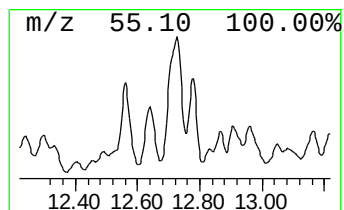
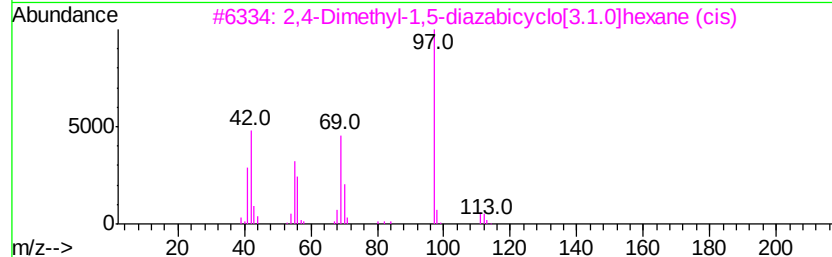
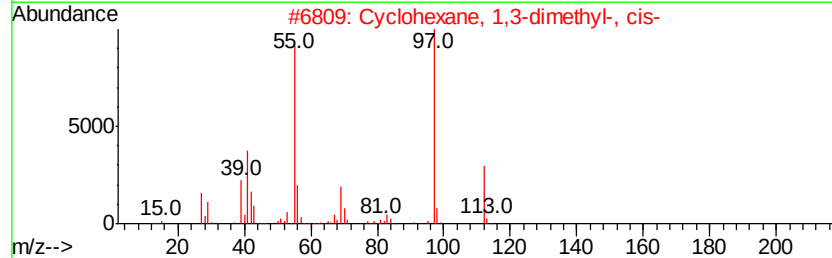
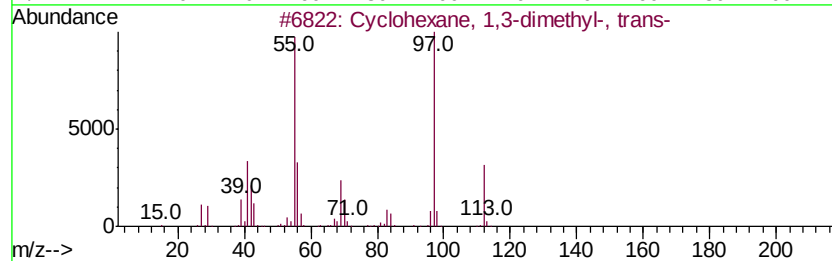
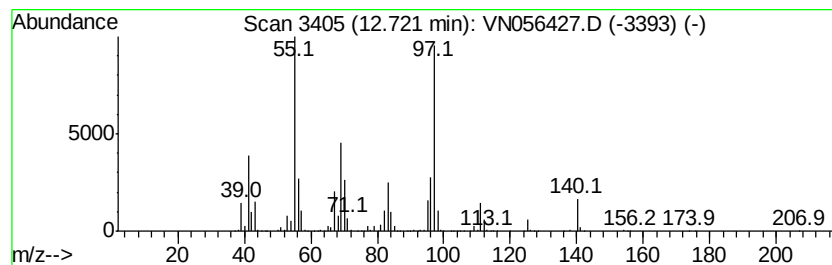
Instrument :
MSVOA_N
ClientSampleId :
TP-3

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N061919W.M
Quant Title : SW846 8260

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

Peak Number 7 Cyclohexane, 1,3-dimethyl-,... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.72	430.67 ug/l	12956700	1,4-Dichlorobenzene-d4	13.34	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,3-dimethyl-, trans-	112	C8H16	002207-03-6	52
2	Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	52
3	2,4-Dimethyl-1,5-diazabicyclo[3.1.0]hexane (cis)	112	C6H12N2	100463-01-2	49
4	2,4-Dimethyl-1,5-diazabicyclo[3.1.0]hexane (trans)	112	C6H12N2	1000283-20-9	49
5	Cyclohexane, 1,1-dimethyl-	112	C8H16	000590-66-9	49



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA N\DATA\VN062119\
Data File : VN056427.D
Acq On : 21 Jun 2019 15:39
Operator : JC/SP
Sample : K3482-05
Misc : 5.19µL/5mL/100µL/5.00mL/MSVOA_N/MEOH
ALS Vial : 18 Sample Multiplier: 1

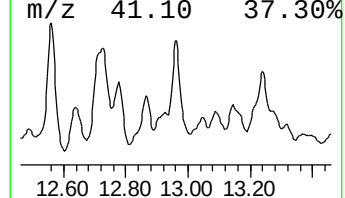
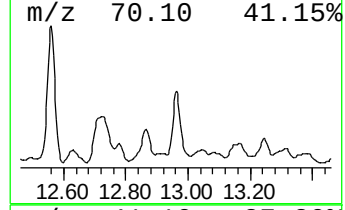
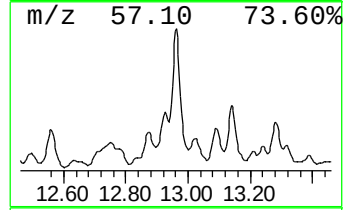
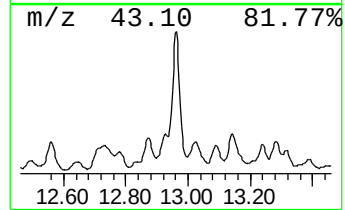
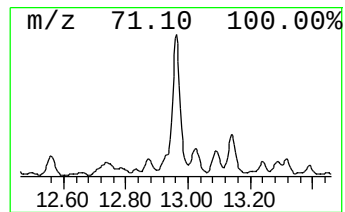
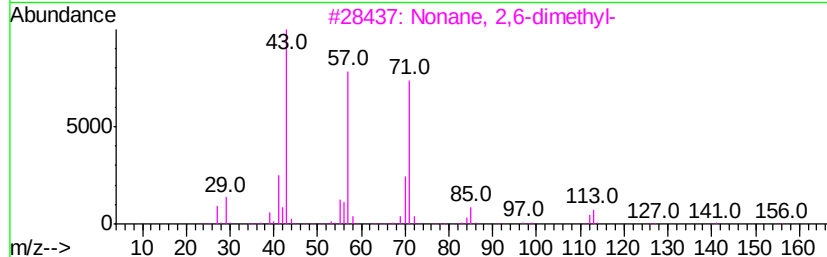
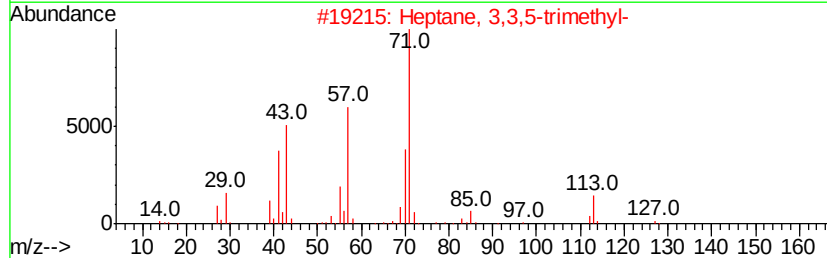
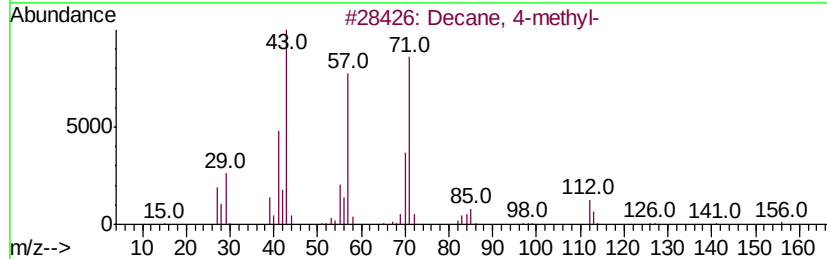
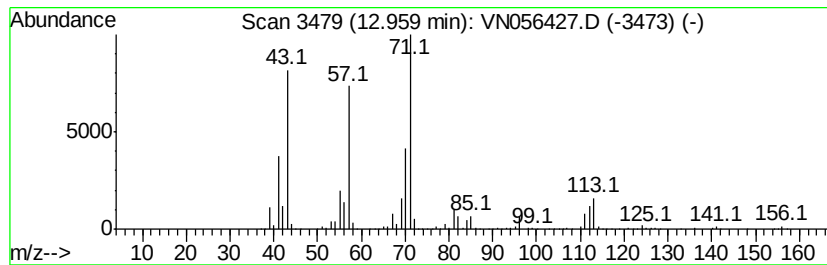
Instrument :
MSVOA_N
ClientSampled :
TP-3

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N061919W.M
Quant Title : SW846 8260

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

Peak Number 8 Decane, 4-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.96	289.63 ug/l	8713500	1,4-Dichlorobenzene-d4	13.34
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Decane, 4-methyl-	156 C11H24	002847-72-5 90
2		Heptane, 3,3,5-trimethyl-	142 C10H22	007154-80-5 78
3		Nonane, 2,6-dimethyl-	156 C11H24	017302-28-2 72
4		Dodecane, 4-methyl-	184 C13H28	006117-97-1 64
5		4-Methyl-3-heptanol, trifluoroac...	226 C10H17F3O2	1000365-51-8 64



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA N\DATA\VN062119\
Data File : VN056427.D
Acq On : 21 Jun 2019 15:39
Operator : JC/SP
Sample : K3482-05
Misc : 5.19µ/5mL/100µL/5.00mL/MSVOA_N/MEOH
ALS Vial : 18 Sample Multiplier: 1

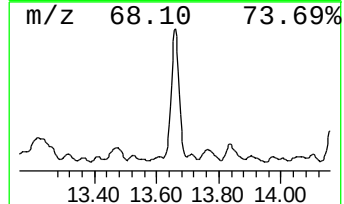
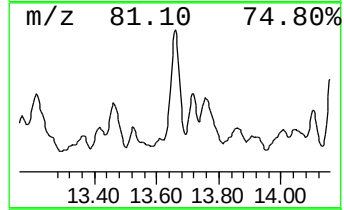
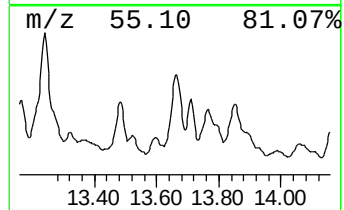
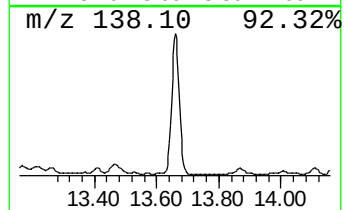
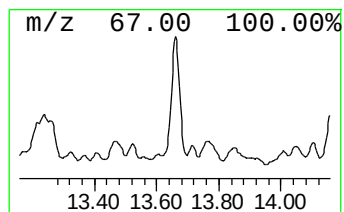
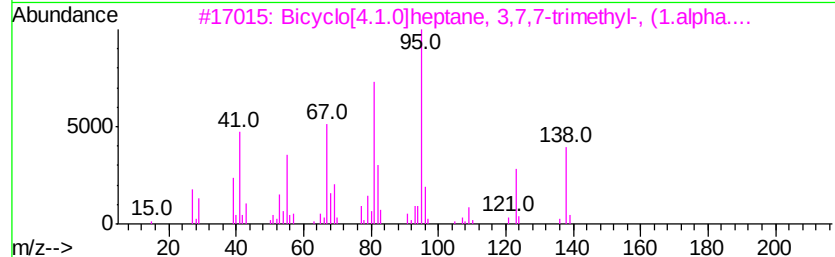
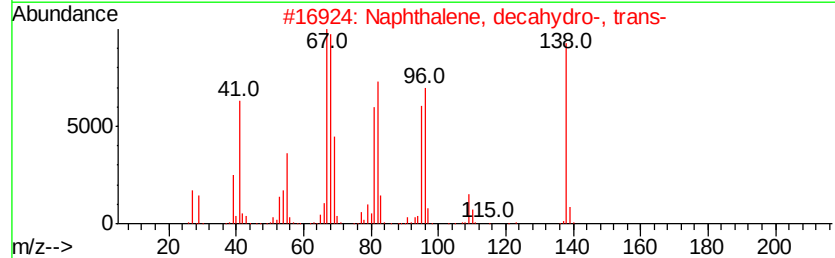
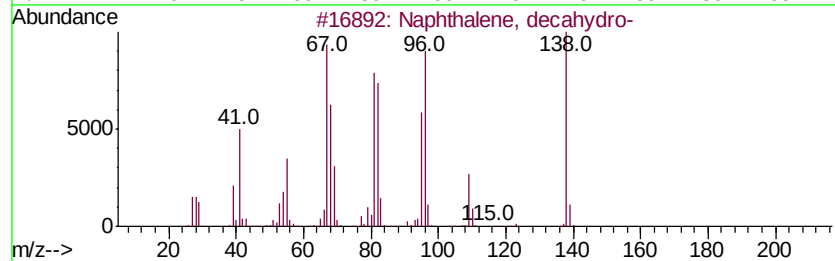
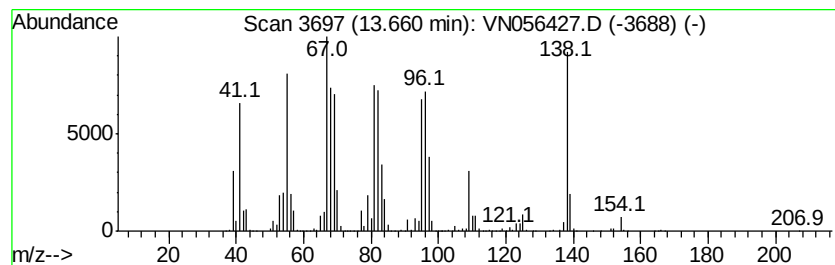
Instrument :
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ClientSampleId :
TP-3

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N061919W.M
Quant Title : SW846 8260

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

Peak Number 9 Naphthalene, decahydro- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.66	285.22 ug/l	8580730	1,4-Dichlorobenzene-d4	13.34
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Naphthalene, decahydro-	138 C10H18	000091-17-8 97
2		Naphthalene, decahydro-, trans-	138 C10H18	000493-02-7 94
3		Bicyclo[4.1.0]heptane, 3,7,7-tri...	138 C10H18	018968-23-5 83
4		Naphthalene, decahydro-, cis-	138 C10H18	000493-01-6 76
5		Spiro[4.5]decane	138 C10H18	000176-63-6 76



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA N\DATA\VN062119\
Data File : VN056427.D
Acq On : 21 Jun 2019 15:39
Operator : JC/SP
Sample : K3482-05
Misc : 5.19µL/5mL/100µL/5.00mL/MSVOA_N/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP-3

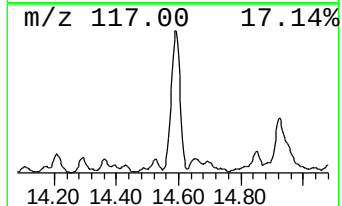
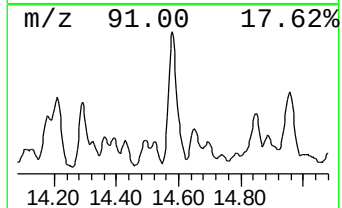
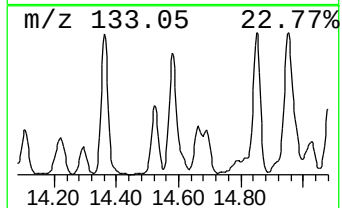
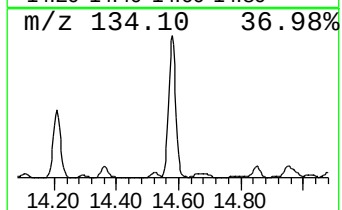
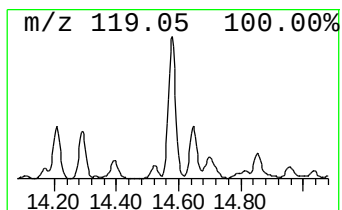
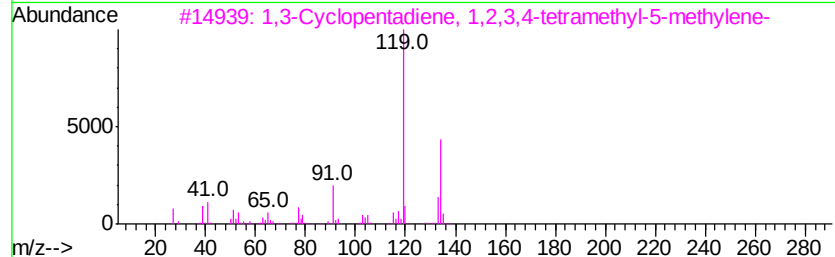
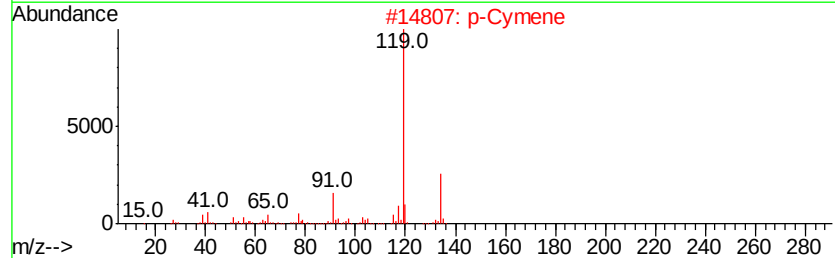
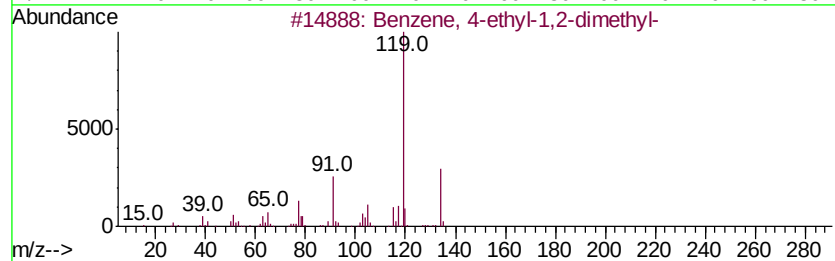
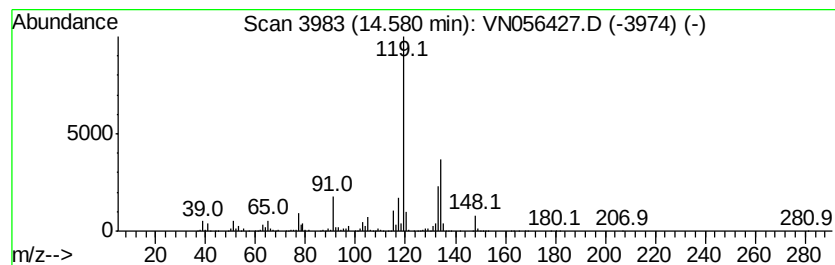
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N061919W.M
Quant Title : SW846 8260

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

Peak Number 10 Benzene, 4-ethyl-1,2-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.58	243.37 ug/l	7321840	1,4-Dichlorobenzene-d4	13.34

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	93
2		p-Cymene	134	C10H14	000099-87-6	87
3		1,3-Cyclopentadiene, 1,2,3,4-tet...	134	C10H14	076089-59-3	87
4		Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	81
5		Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	81



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN062119\
Data File : VN056427.D
Acq On : 21 Jun 2019 15:39
Operator : JC/SP
Sample : K3482-05
Misc : 5.19g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP-3

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N061919W.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Cyclohexane, 1,1,...	11.00	414.9	ug/l	11747300	3	11.41	1415740	50.0
Cyclohexane, 1,2,...	11.20	313.1	ug/l	8866310	3	11.41	1415740	50.0
1-Ethyl-4-methylc...	11.65	215.3	ug/l	6096650	3	11.41	1415740	50.0
Cyclohexane, 1-et...	11.92	366.9	ug/l	10387700	3	11.41	1415740	50.0
Cyclohexane, propyl-	12.16	352.2	ug/l	9971930	3	11.41	1415740	50.0
2-Octene, 2,6-dim...	12.56	396.5	ug/l	11929800	4	13.34	1504250	50.0
Cyclohexane, 1,3-...	12.72	430.7	ug/l	12956700	4	13.34	1504250	50.0
Decane, 4-methyl-	12.96	289.6	ug/l	8713500	4	13.34	1504250	50.0
Naphthalene, deca...	13.66	285.2	ug/l	8580730	4	13.34	1504250	50.0
Benzene, 4-ethyl-...	14.58	243.4	ug/l	7321840	4	13.34	1504250	50.0