

Data Path : Z:\voasrv\HPCHEM1\MSVOA N\Data\VN032219\
 Data File : VN054552.D
 Acq On : 22 Mar 2019 12:35
 Operator : JC/SP
 Sample : K2004-03
 Misc : 4.80g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 SB-19(7.5-8.5)

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\82N032019W.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	2.494	203	224	225	rBV3	32017	73883	2.00%	0.103%
2	2.561	238	245	257	rVB3	63893	117103	3.18%	0.164%
3	6.506	1457	1472	1489	rBV4	22445	66774	1.81%	0.094%
4	7.590	1789	1809	1819	rBV2	359182	886401	24.03%	1.241%
5	7.660	1819	1831	1845	rVV	661579	1615914	43.81%	2.263%
6	7.734	1847	1854	1874	rVB3	107682	271548	7.36%	0.380%
7	7.924	1902	1913	1928	rVB5	37262	91698	2.49%	0.128%
8	8.024	1929	1944	1966	rBV	415168	951753	25.81%	1.333%
9	8.143	1967	1981	1994	rBV5	46088	111415	3.02%	0.156%
10	8.583	2103	2118	2143	rVB	972489	2061791	55.90%	2.887%
11	8.895	2200	2215	2231	rVB	66374	152740	4.14%	0.214%
12	9.043	2239	2261	2267	rBV2	270295	577951	15.67%	0.809%
13	9.085	2268	2274	2283	rVV	350568	655881	17.78%	0.918%
14	9.140	2283	2291	2307	rVV2	238744	470323	12.75%	0.659%
15	9.361	2337	2360	2381	rBV2	370667	1034648	28.05%	1.449%
16	9.513	2394	2407	2419	rVB5	28740	58963	1.60%	0.083%
17	9.664	2437	2454	2478	rBV	282788	628292	17.04%	0.880%
18	9.840	2492	2509	2518	rBV3	265432	550367	14.92%	0.771%
19	9.895	2518	2526	2540	rVB	348035	647980	17.57%	0.907%
20	9.976	2540	2551	2556	rBV2	70360	133157	3.61%	0.186%
21	10.088	2573	2586	2617	rBV	1525795	3541271	96.02%	4.959%
22	10.252	2618	2637	2657	rVB	570915	1281305	34.74%	1.794%
23	10.394	2661	2681	2683	rBV4	140014	275275	7.46%	0.385%
24	10.429	2684	2692	2710	rVB	670831	1242248	33.68%	1.739%
25	10.529	2710	2723	2731	rBV2	436796	910948	24.70%	1.276%
26	10.577	2732	2738	2745	rVV2	276136	441873	11.98%	0.619%
27	10.625	2745	2753	2763	rVB	459016	742636	20.14%	1.040%
28	10.818	2799	2813	2827	rBV	1099802	2306563	62.54%	3.230%
29	10.889	2827	2835	2857	rVB3	510382	1195701	32.42%	1.674%
30	11.004	2858	2871	2881	rBV2	1177412	2194115	59.49%	3.072%
31	11.059	2881	2888	2897	rVV	376993	629529	17.07%	0.882%
32	11.123	2897	2908	2914	rVV2	497630	916183	24.84%	1.283%
33	11.162	2914	2920	2927	rVV2	626486	1058564	28.70%	1.482%
34	11.210	2927	2935	2951	rVB	1046720	1965279	53.29%	2.752%

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35	11.287	2951	2959	2969	rBV	370408	587878	15.94%	0.823%
36	11.406	2983	2996	3013	rBV	1263421	2481465	67.28%	3.475%
37	11.541	3029	3038	3045	rBV	336280	533263	14.46%	0.747%
38	11.596	3046	3055	3062	rBV4	295865	529426	14.36%	0.741%
39	11.654	3062	3073	3081	rVV	1385465	2543866	68.98%	3.562%
40	11.696	3082	3086	3097	rVB2	763811	1126423	30.54%	1.577%
41	11.754	3099	3104	3108	rBV5	30484	39041	1.06%	0.055%
42	11.808	3109	3121	3127	rBV4	259959	632496	17.15%	0.886%
43	11.850	3127	3134	3143	rVB3	468883	725536	19.67%	1.016%
44	11.921	3143	3156	3169	rBV8	1430121	3688068	100.00%	5.164%
45	12.114	3200	3216	3223	rBV5	887438	2135286	57.90%	2.990%
46	12.162	3224	3231	3241	rVB4	771097	1409599	38.22%	1.974%
47	12.294	3260	3272	3283	rVB5	928965	2122197	57.54%	2.972%
48	12.403	3294	3306	3317	rBV2	1226487	2332127	63.23%	3.266%
49	12.644	3370	3381	3392	rBV5	415119	1004735	27.24%	1.407%
50	12.728	3394	3407	3416	rVV2	1361225	2875560	77.97%	4.027%
51	12.779	3416	3423	3433	rVB2	789305	1341738	36.38%	1.879%
52	12.866	3444	3450	3457	rBV3	334174	444883	12.06%	0.623%
53	12.927	3458	3469	3473	rVV5	336277	727086	19.71%	1.018%
54	12.959	3474	3479	3492	rVB4	647930	1112542	30.17%	1.558%
55	13.088	3512	3519	3530	rVB4	305496	504209	13.67%	0.706%
56	13.239	3551	3566	3574	rBV2	1235325	2352080	63.78%	3.294%
57	13.342	3589	3598	3625	rVB	1165928	2332636	63.25%	3.266%
58	13.660	3687	3697	3706	rBV4	866892	1567871	42.51%	2.195%
59	13.709	3707	3712	3720	rVB	409317	569061	15.43%	0.797%
60	13.770	3723	3731	3744	rVB4	392391	714674	19.38%	1.001%
61	14.178	3846	3858	3878	rBV7	919626	2255576	61.16%	3.158%
62	14.332	3898	3906	3914	rBV	427174	675611	18.32%	0.946%
63	14.593	3979	3987	3995	rBV3	269495	469775	12.74%	0.658%
64	14.641	3995	4002	4014	rVB4	469538	808735	21.93%	1.132%
65	15.043	4119	4127	4139	rVB4	394110	726827	19.71%	1.018%
66	15.114	4143	4149	4157	rVV2	133063	184225	5.00%	0.258%

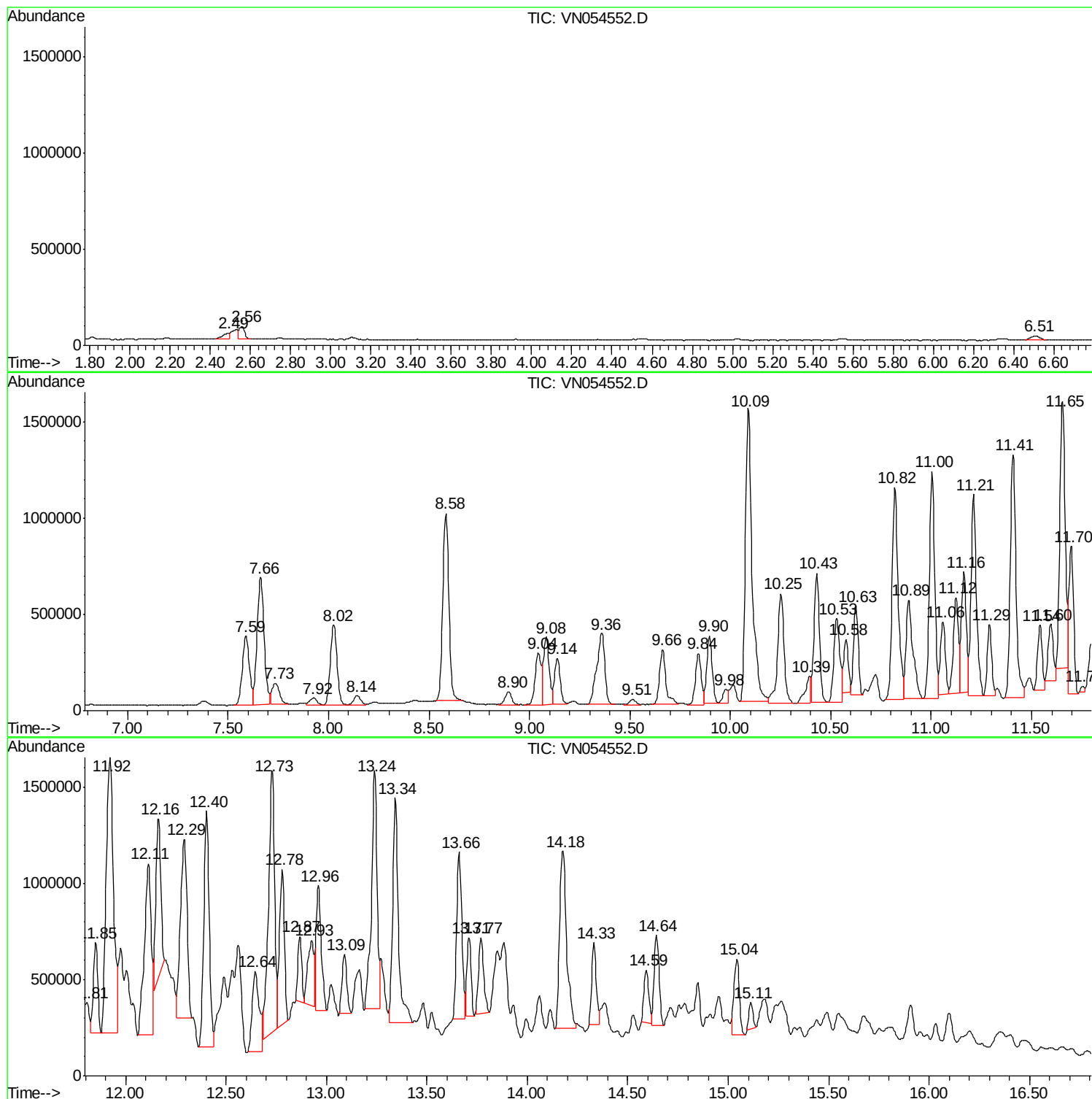
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ClientSampleId :
SB-19(7.5-8.5)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N032019W.M
Quant Title : SW846 8260

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



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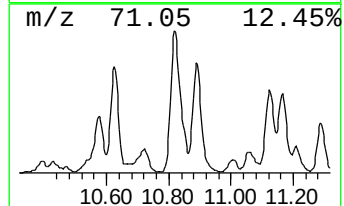
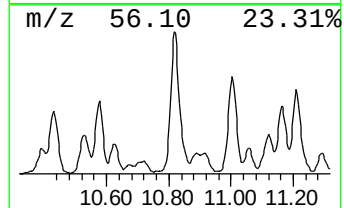
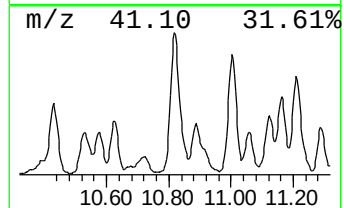
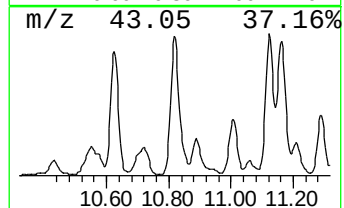
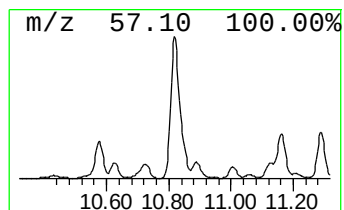
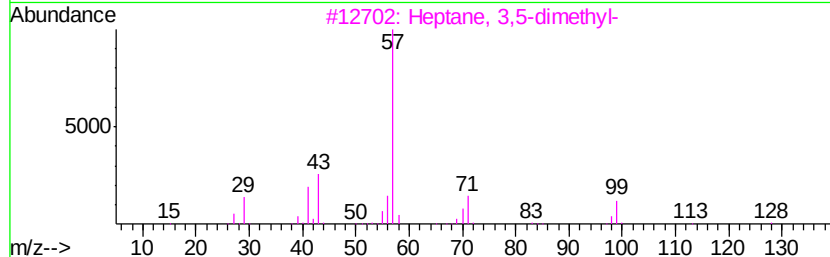
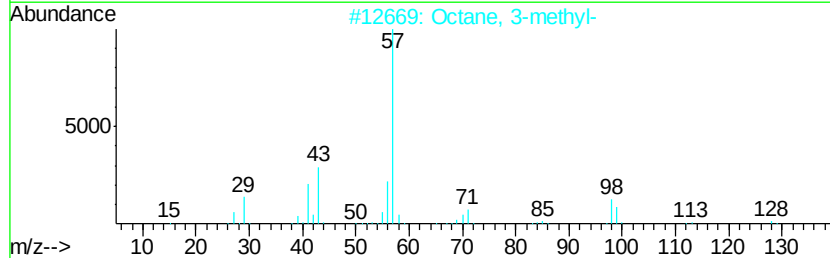
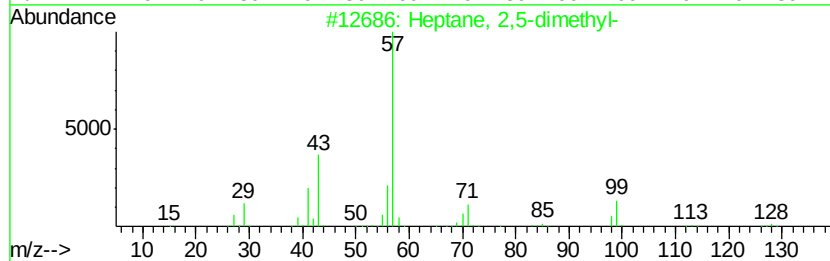
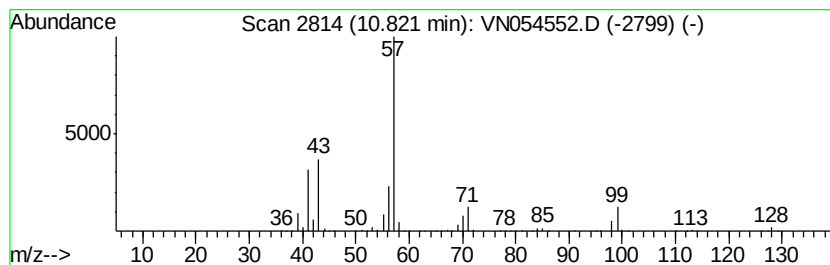
Instrument :
MSVOA_N
ClientSampleId :
SB-19(7.5-8.5)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N032019W.M
Quant Title : SW846 8260

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

Peak Number 1 Heptane, 2,5-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.82	46.48 ug/l	2306560	Chlorobenzene-d5	11.41	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane, 2,5-dimethyl-	128	C9H20	002216-30-0	91
2	Octane, 3-methyl-	128	C9H20	002216-33-3	90
3	Heptane, 3,5-dimethyl-	128	C9H20	000926-82-9	81
4	Decane, 2,6,6-trimethyl-	184	C13H28	062108-24-1	59
5	Heptane, 2,3,5-trimethyl-	142	C10H22	020278-85-7	47



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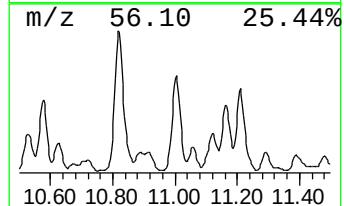
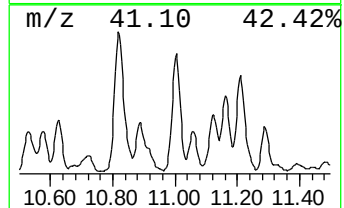
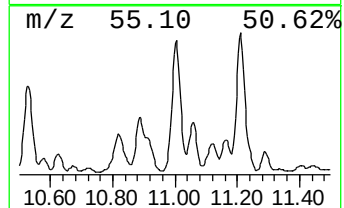
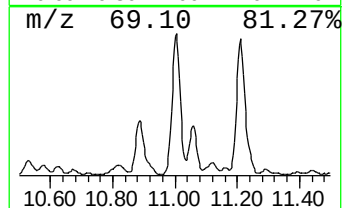
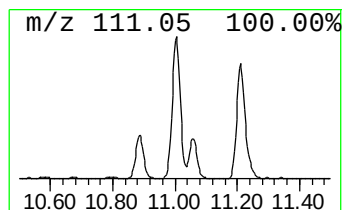
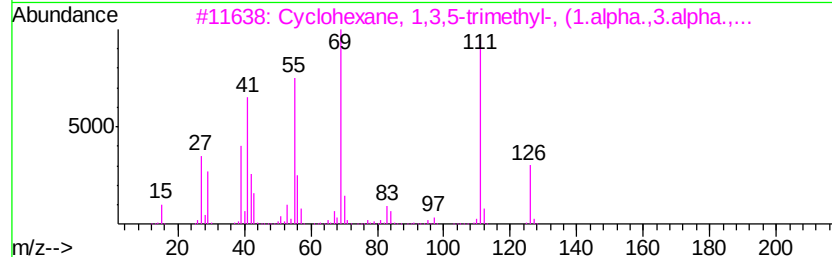
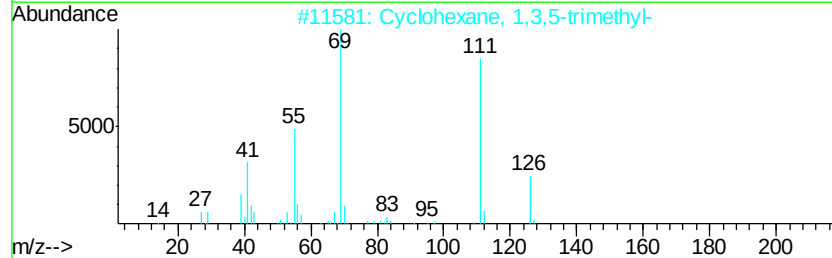
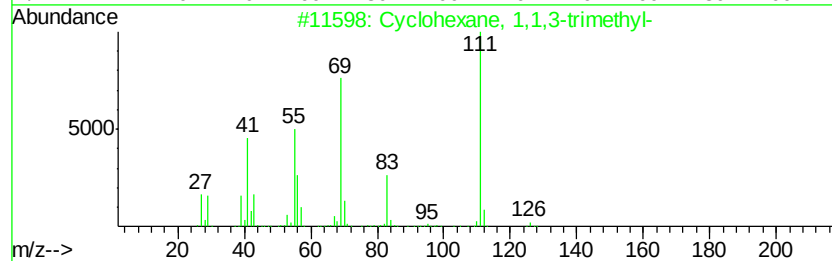
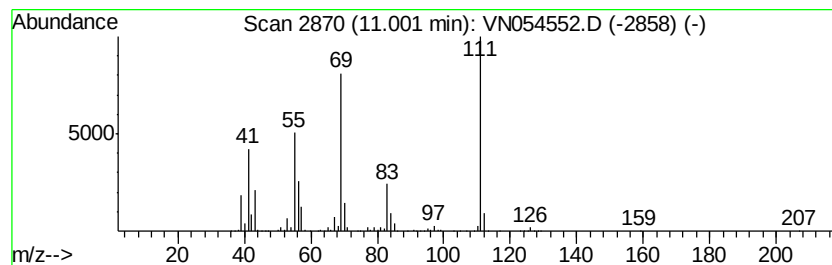
Instrument :
MSVOA_N
ClientSampled :
SB-19(7.5-8.5)

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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 Cyclohexane, 1,1,3-trimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.00	44.21 ug/l	2194120	Chlorobenzene-d5	11.41	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,1,3-trimethyl-	126	C9H18	003073-66-3	95
2	Cyclohexane, 1,3,5-trimethyl-	126	C9H18	001839-63-0	64
3	Cyclohexane, 1,3,5-trimethyl-, (...)	126	C9H18	001795-26-2	64
4	Cyclohexane, 1,3,5-trimethyl-, (...)	126	C9H18	001795-27-3	64
5	1-Hexene, 3,3-dimethyl-	112	C8H16	003404-77-1	46



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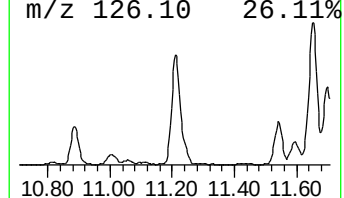
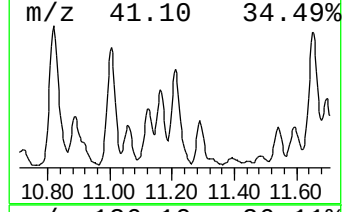
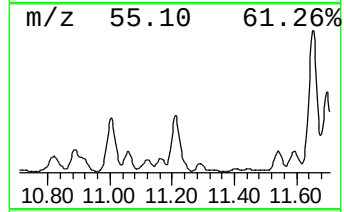
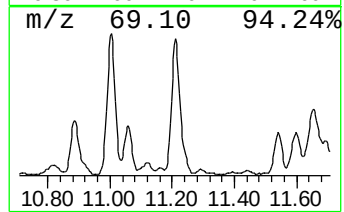
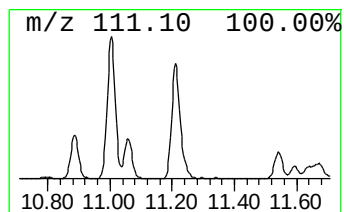
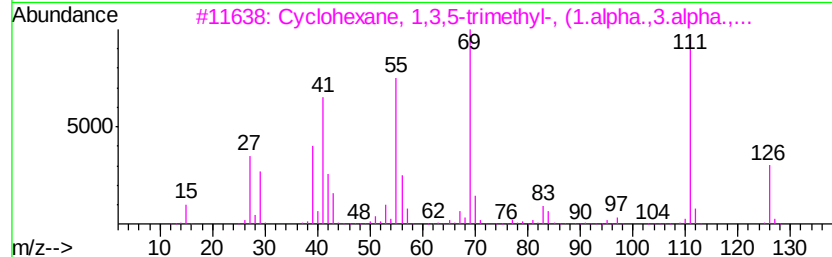
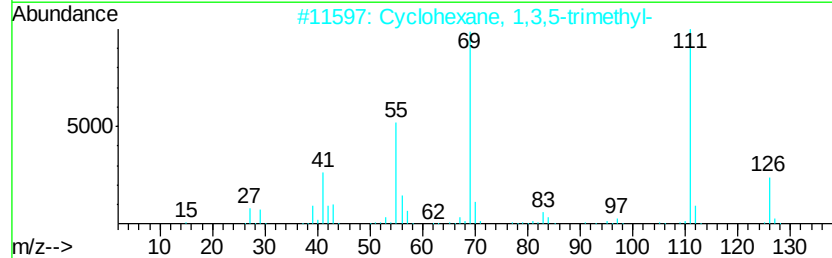
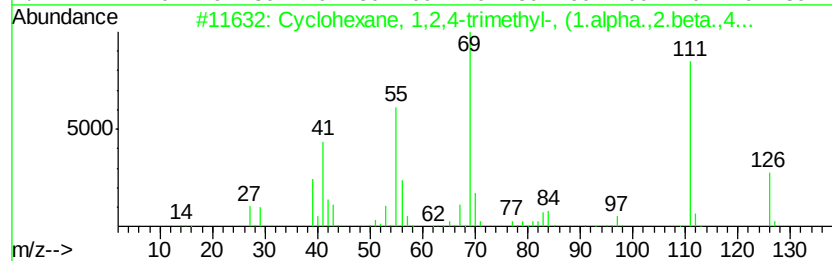
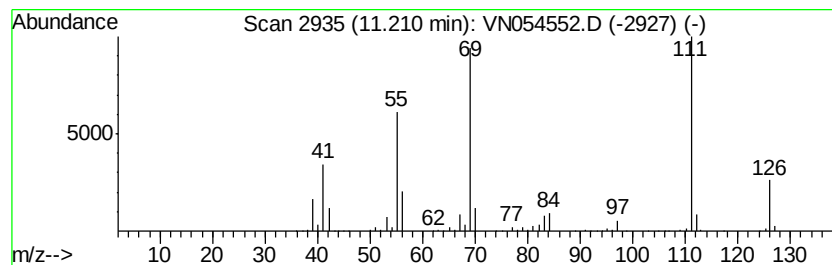
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TIC Integration Parameters: LSCINT.P

Peak Number 3 Cyclohexane, 1,2,4-trimethy... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.21	39.60 ug/l	1965280	Chlorobenzene-d5	11.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, 1,2,4-trimethyl-, (...)	126	C9H18	007667-60-9	94
2		Cyclohexane, 1,3,5-trimethyl-	126	C9H18	001839-63-0	93
3		Cyclohexane, 1,3,5-trimethyl-, (...)	126	C9H18	001795-26-2	93
4		Cyclohexane, 1,3,5-trimethyl-, (...)	126	C9H18	001795-27-3	90
5		Cyclooctane, (1-methylpropyl)-	168	C12H24	016538-89-9	64



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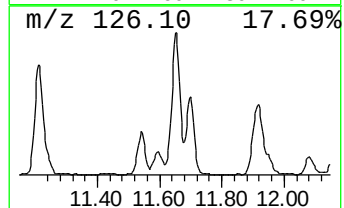
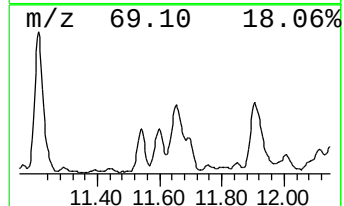
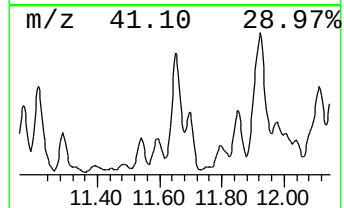
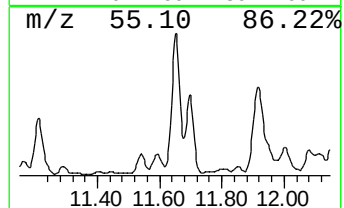
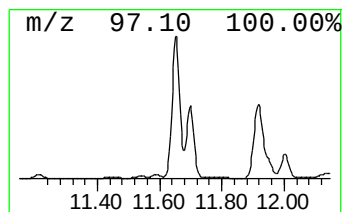
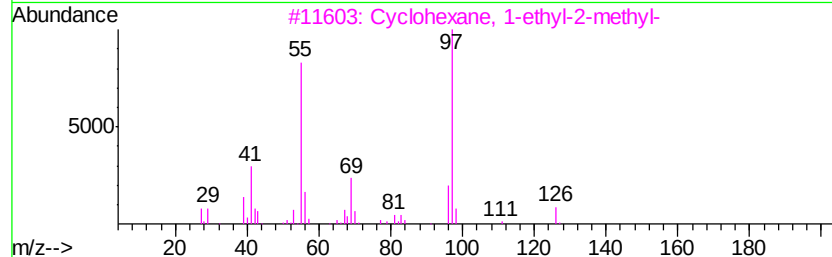
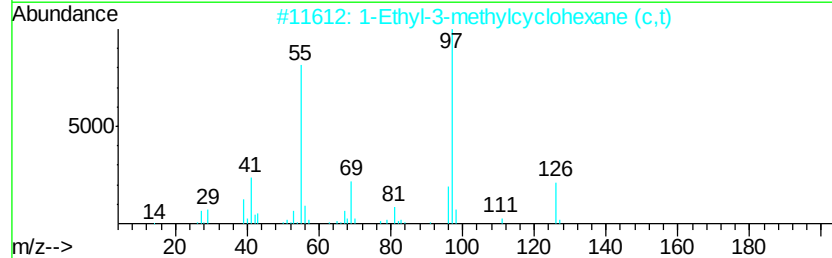
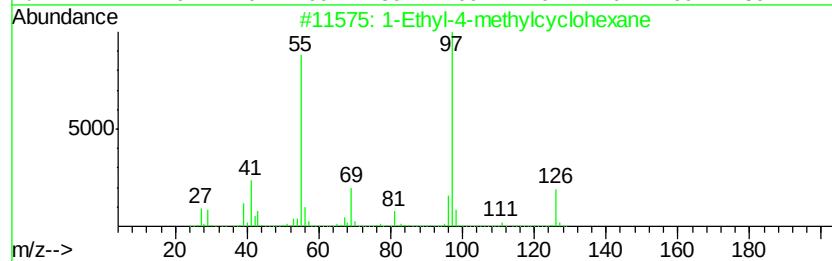
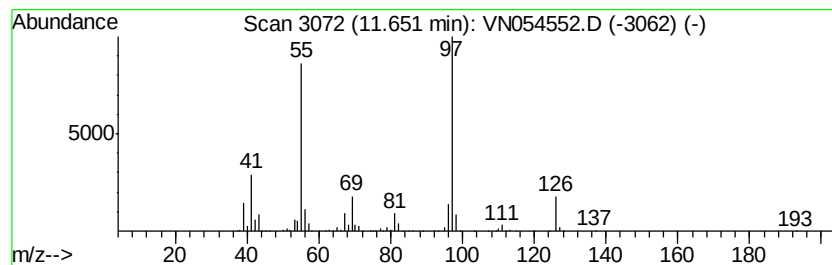
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Peak Number 4 1-Ethyl-4-methylcyclohexane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.65	51.26 ug/l	2543870	Chlorobenzene-d5	11.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Ethyl-4-methylcyclohexane	126	C9H18	003728-56-1	95
2		1-Ethyl-3-methylcyclohexane (c,t)	126	C9H18	003728-55-0	94
3		Cyclohexane, 1-ethyl-2-methyl-	126	C9H18	003728-54-9	91
4		cis-1-Ethyl-3-methyl-cyclohexane	126	C9H18	019489-10-2	90
5		Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	006236-88-0	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA N\Data\VN032219\
Data File : VN054552.D
Acq On : 22 Mar 2019 12:35
Operator : JC/SP
Sample : K2004-03
Misc : 4.80g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

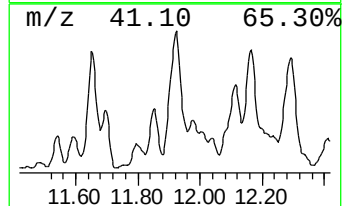
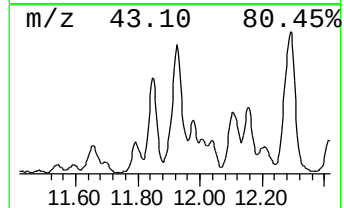
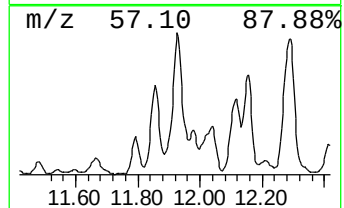
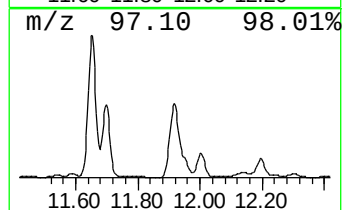
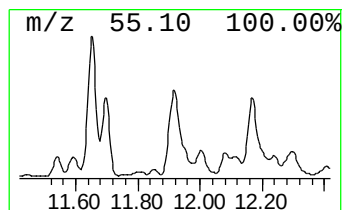
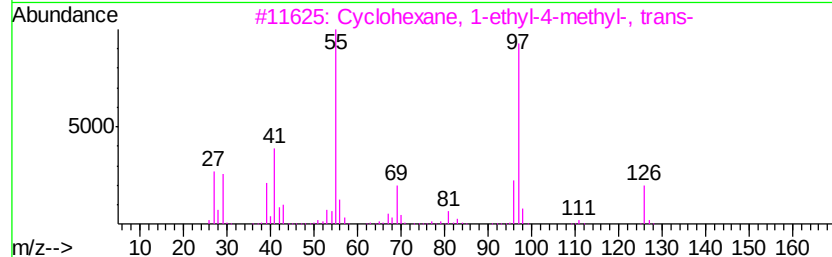
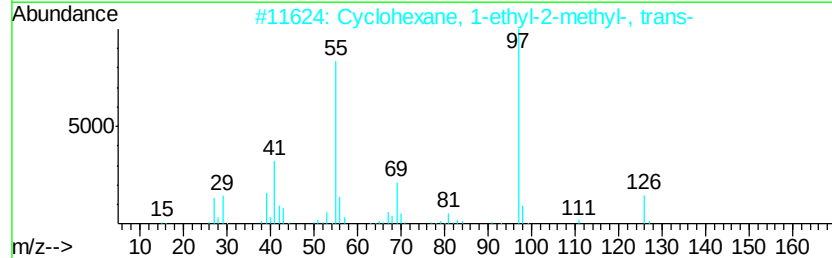
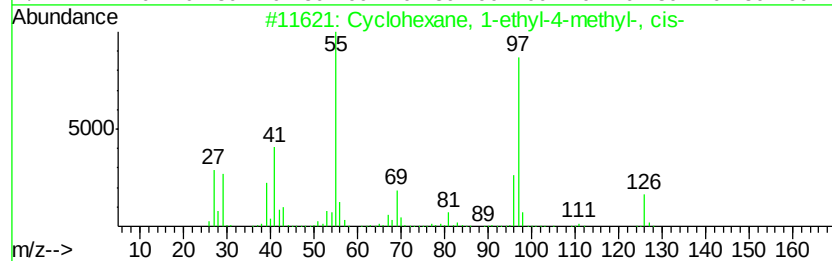
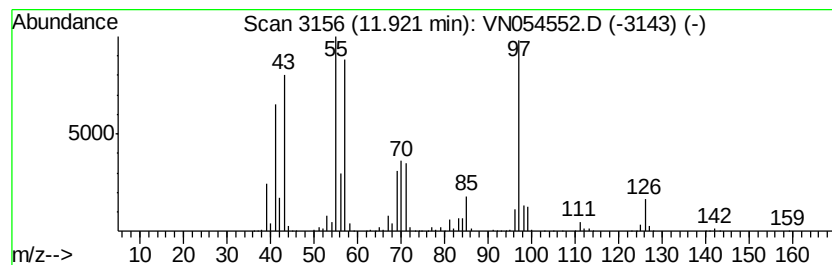
Instrument :
MSVOA_N
ClientSampleId :
SB-19(7.5-8.5)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N032019W.M
Quant Title : SW846 8260

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

Peak Number 5 unknown11.92 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.92	74.31 ug/l	3688070	Chlorobenzene-d5	11.41	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	004926-78-7	46
2	Cyclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-78-8	46
3	Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	006236-88-0	46
4	Cyclohexane, 1-ethyl-2-methyl-	126	C9H18	003728-54-9	46
5	2-Hexene, 3,4,4-trimethyl-	126	C9H18	053941-19-8	46



Data Path : Z:\voasrv\HPCHEM1\MSVOA N\Data\VN032219\
Data File : VN054552.D
Acq On : 22 Mar 2019 12:35
Operator : JC/SP
Sample : K2004-03
Misc : 4.80g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SB-19(7.5-8.5)

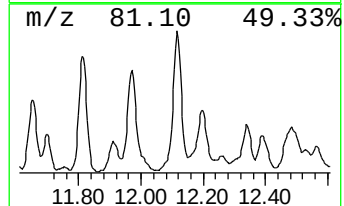
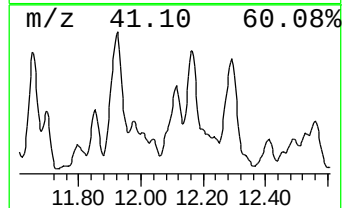
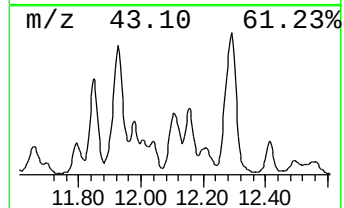
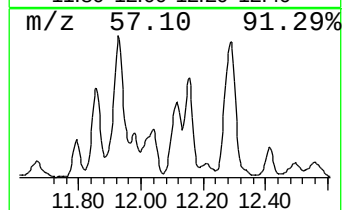
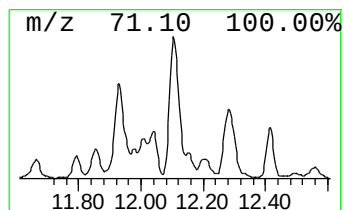
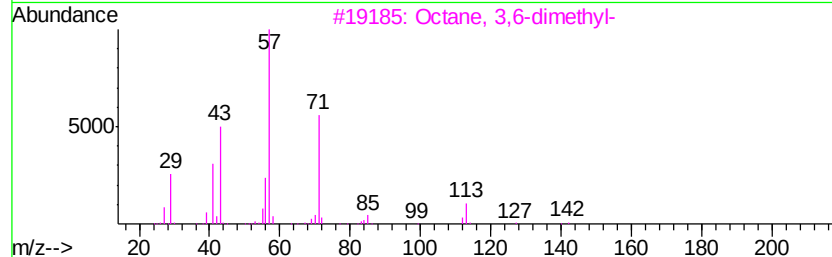
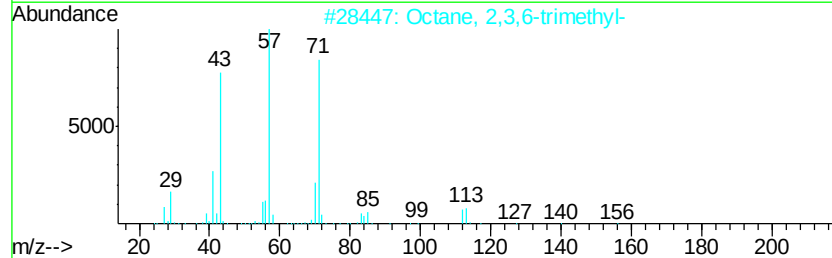
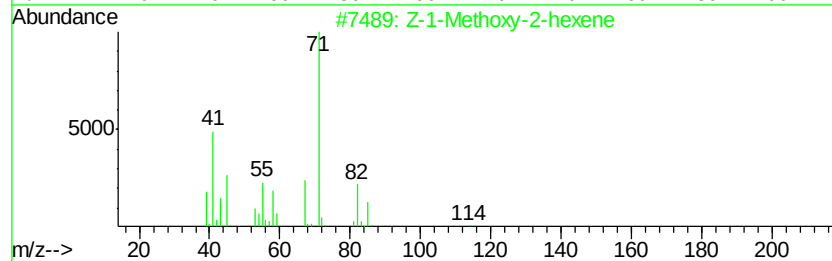
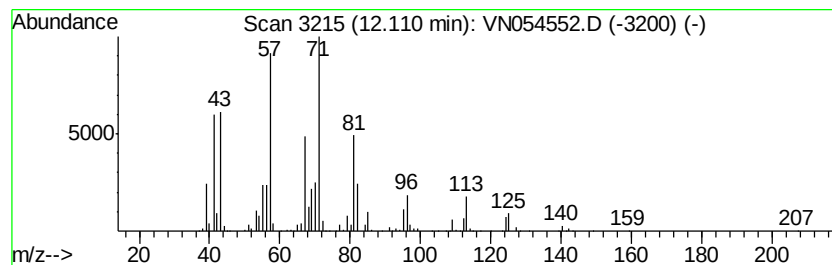
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Quant Title : SW846 8260

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

Peak Number 6 unknown12.11 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.11	43.02 ug/l	2135290	Chlorobenzene-d5	11.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Z-1-Methoxy-2-hexene	114	C7H14O	1000279-60-9	43
2		Octane, 2,3,6-trimethyl-	156	C11H24	062016-33-5	43
3		Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	30
4		Nonane, 3-methyl-	142	C10H22	005911-04-6	30
5		Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	25



Data Path : Z:\voasrv\HPCHEM1\MSVOA N\Data\VN032219\
Data File : VN054552.D
Acq On : 22 Mar 2019 12:35
Operator : JC/SP
Sample : K2004-03
Misc : 4.80g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

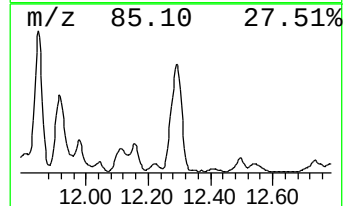
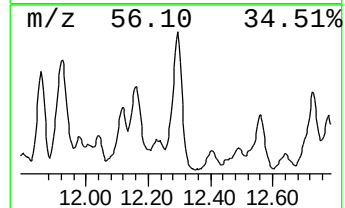
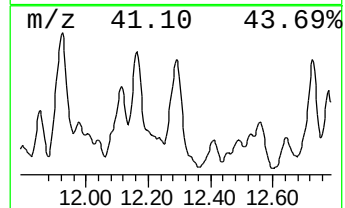
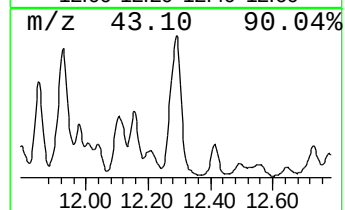
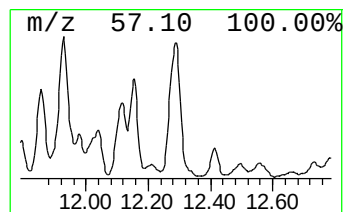
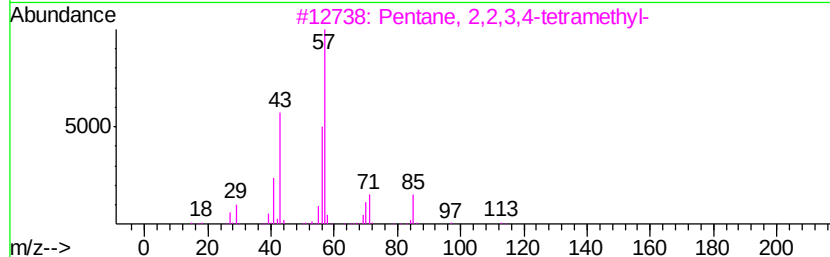
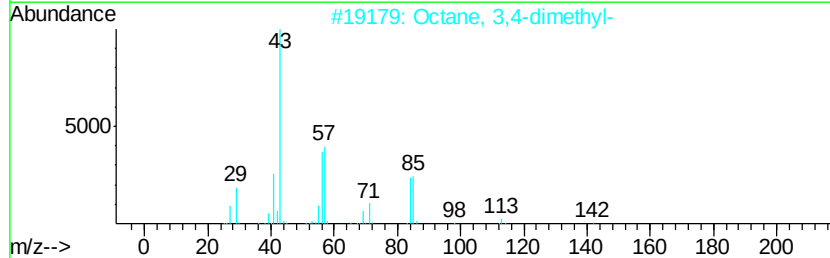
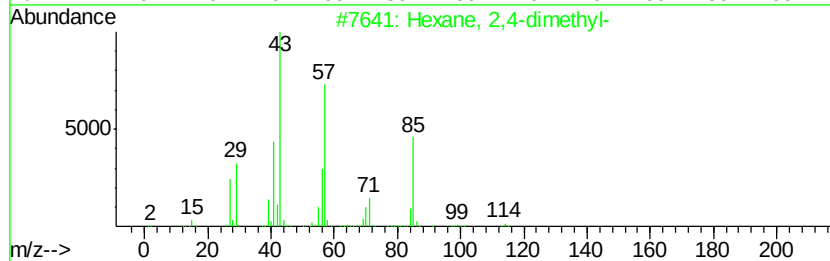
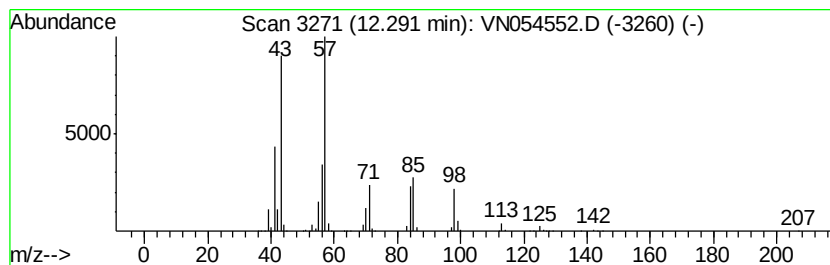
Instrument :
MSVOA_N
ClientSampleId :
SB-19(7.5-8.5)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N032019W.M
Quant Title : SW846 8260

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

Peak Number 7 Hexane, 2,4-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.29	42.76 ug/l	2122200	Chlorobenzene-d5	11.41
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Hexane, 2,4-dimethyl-	114 C8H18	000589-43-5	58
2	Octane, 3,4-dimethyl-	142 C10H22	015869-92-8	53
3	Pentane, 2,2,3,4-tetramethyl-	128 C9H20	001186-53-4	47
4	Heptane, 2,3-dimethyl-	128 C9H20	003074-71-3	43
5	Heptane, 4-ethyl-	128 C9H20	002216-32-2	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA N\Data\VN032219\
Data File : VN054552.D
Acq On : 22 Mar 2019 12:35
Operator : JC/SP
Sample : K2004-03
Misc : 4.80g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

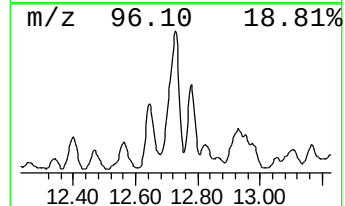
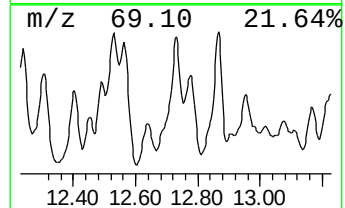
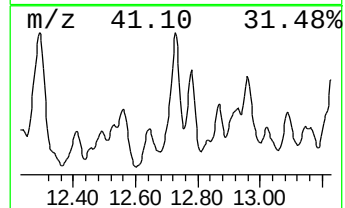
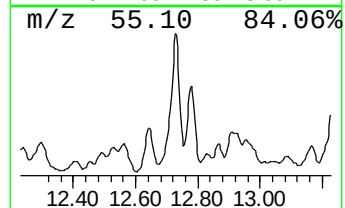
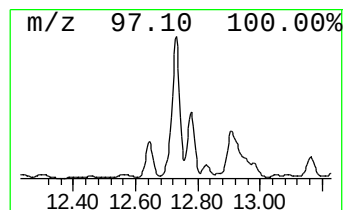
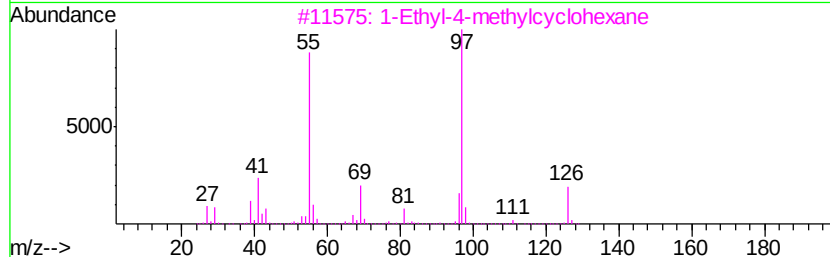
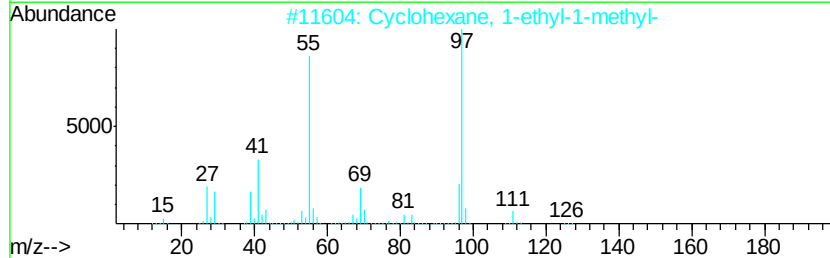
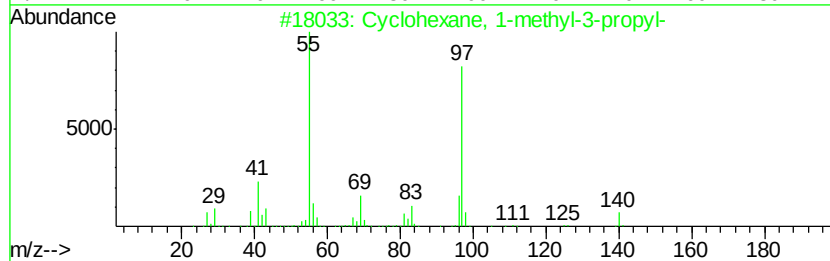
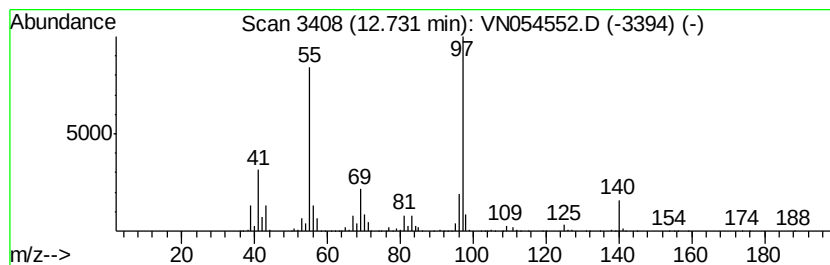
Instrument :
MSVOA_N
ClientSampled :
SB-19(7.5-8.5)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N032019W.M
Quant Title : SW846 8260

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

Peak Number 8 Cyclohexane, 1-methyl-3-pro... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.73	61.64 ug/l	2875560	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 90
2		Cyclohexane, 1-ethyl-1-methyl-	126 C9H18	004926-90-3 90
3		1-Ethyl-4-methylcyclohexane	126 C9H18	003728-56-1 87
4		Cyclohexane, 1-methyl-2-propyl-	140 C10H20	004291-79-6 87
5		Cyclohexane, 1-methyl-4-(1-methy...	140 C10H20	006069-98-3 81



Data Path : Z:\voasrv\HPCHEM1\MSVOA N\Data\VN032219\
Data File : VN054552.D
Acq On : 22 Mar 2019 12:35
Operator : JC/SP
Sample : K2004-03
Misc : 4.80g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

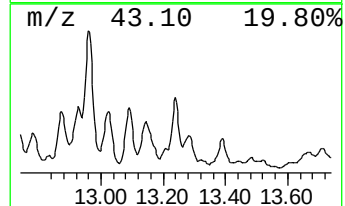
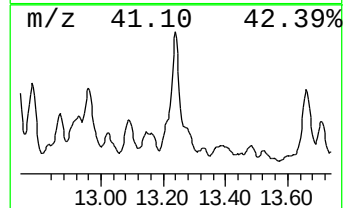
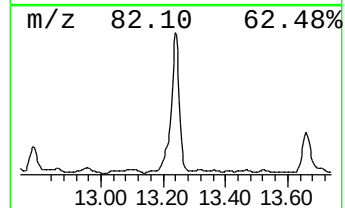
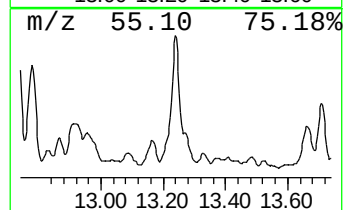
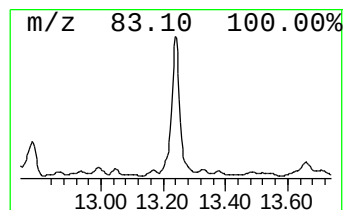
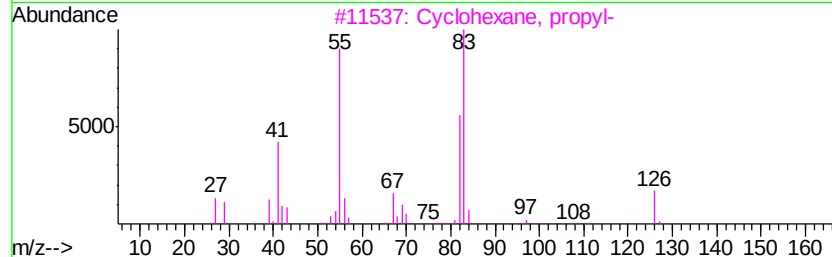
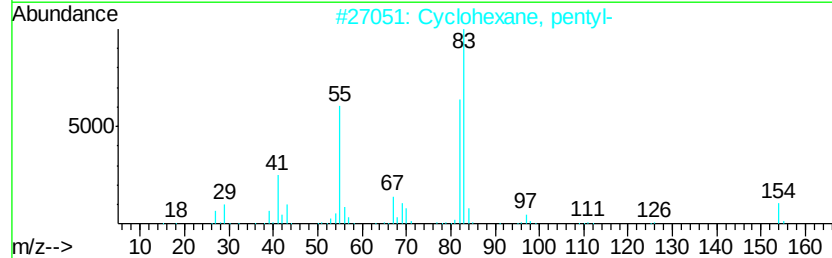
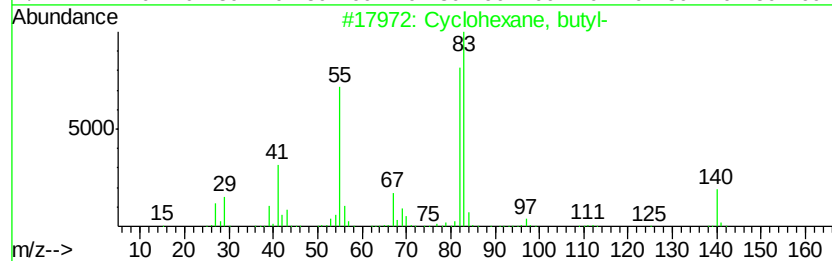
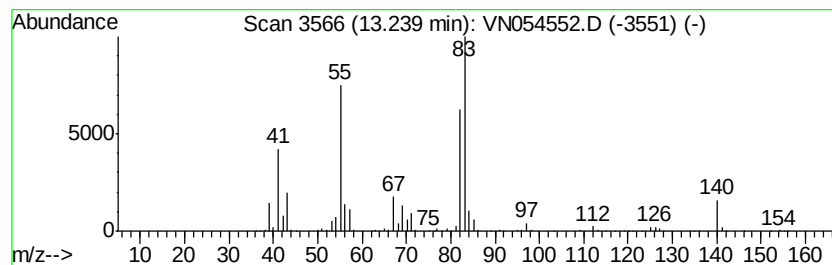
Instrument :
MSVOA_N
ClientSampleId :
SB-19(7.5-8.5)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N032019W.M
Quant Title : SW846 8260

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

Peak Number 9 Cyclohexane, butyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.24	50.42 ug/l	2352080	1,4-Dichlorobenzene-d4	13.35	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, butyl-	140	C10H20	001678-93-9	95
2	Cyclohexane, pentyl-	154	C11H22	004292-92-6	87
3	Cyclohexane, propyl-	126	C9H18	001678-92-8	87
4	Cyclohexane, (2-methylpropyl)-	140	C10H20	001678-98-4	83
5	Cyclohexane, ethyl-	112	C8H16	001678-91-7	80



Data Path : Z:\voasrv\HPCHEM1\MSVOA N\Data\VN032219\
Data File : VN054552.D
Acq On : 22 Mar 2019 12:35
Operator : JC/SP
Sample : K2004-03
Misc : 4.80g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

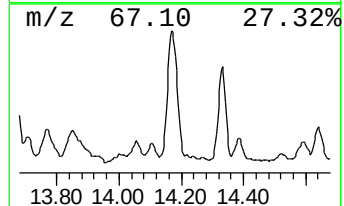
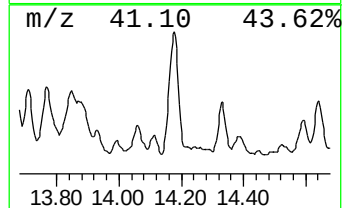
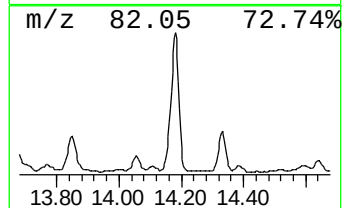
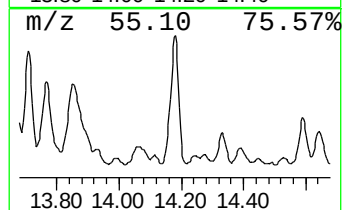
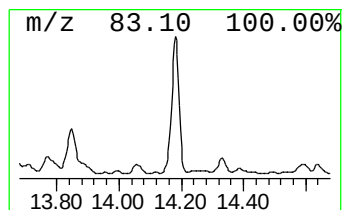
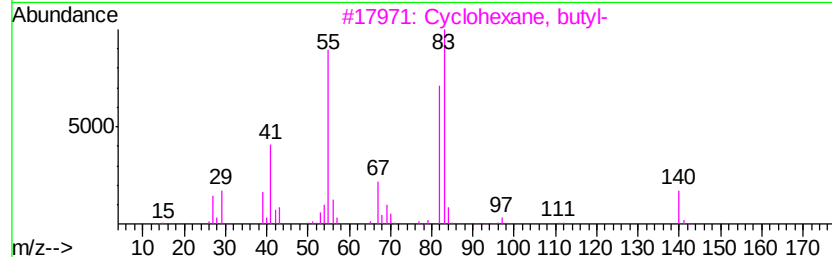
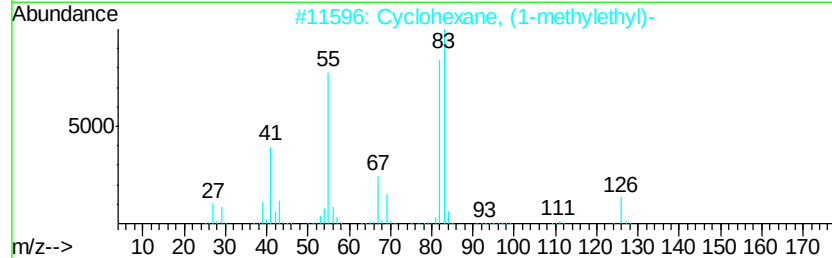
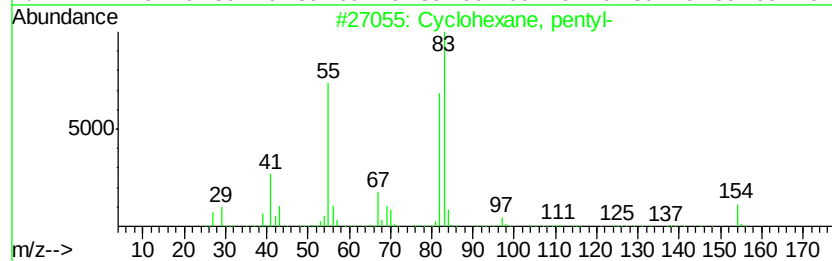
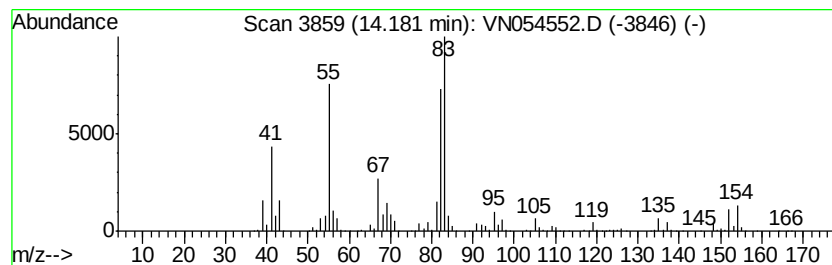
Instrument :
MSVOA_N
ClientSampleId :
SB-19(7.5-8.5)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N032019W.M
Quant Title : SW846 8260

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

Peak Number 10 Cyclohexane, pentyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.18	48.35 ug/l	2255580	1,4-Dichlorobenzene-d4	13.35	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, pentyl-	154	C11H22	004292-92-6	81
2	Cyclohexane, (1-methylethyl)-	126	C9H18	000696-29-7	81
3	Cyclohexane, butyl-	140	C10H20	001678-93-9	64
4	Cyclohexane, propyl-	126	C9H18	001678-92-8	59
5	Cyclohexane, (1-methylbutyl)-	154	C11H22	061208-94-4	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN032219\
Data File : VN054552.D
Acq On : 22 Mar 2019 12:35
Operator : JC/SP
Sample : K2004-03
Misc : 4.80g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SB-19(7.5-8.5)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N032019W.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
Heptane, 2,5-dime...	10.82	46.5	ug/l	2306560	3	11.41	2481470	50.0
Cyclohexane, 1,1,...	11.00	44.2	ug/l	2194120	3	11.41	2481470	50.0
Cyclohexane, 1,2,...	11.21	39.6	ug/l	1965280	3	11.41	2481470	50.0
1-Ethyl-4-methylc...	11.65	51.3	ug/l	2543870	3	11.41	2481470	50.0
unknown11.92	11.92	74.3	ug/l	3688070	3	11.41	2481470	50.0
unknown12.11	12.11	43.0	ug/l	2135290	3	11.41	2481470	50.0
Hexane, 2,4-dimet...	12.29	42.8	ug/l	2122200	3	11.41	2481470	50.0
Cyclohexane, 1-me...	12.73	61.6	ug/l	2875560	4	13.35	2332640	50.0
Cyclohexane, butyl-	13.24	50.4	ug/l	2352080	4	13.35	2332640	50.0
Cyclohexane, pentyl-	14.18	48.4	ug/l	2255580	4	13.35	2332640	50.0