

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN050319\
 Data File : VN055380.D
 Acq On : 3 May 2019 11:12
 Operator : JC/SP
 Sample : K2658-08 10X
 Misc : 5.17g/5mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 EP1-SB-E3-4(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\82N042919W.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	7.593	1785	1810	1821	rBV2	306444	777525	2.86%	0.289%
2	7.667	1821	1833	1855	rVB	492975	1184817	4.35%	0.440%
3	8.027	1928	1945	1974	rBV	335073	808343	2.97%	0.300%
4	8.587	2102	2119	2151	rBV	795740	1776296	6.53%	0.660%
5	10.088	2572	2586	2617	rBV3	1469784	3219270	11.83%	1.196%
6	10.432	2684	2693	2709	rVB2	263290	498565	1.83%	0.185%
7	10.532	2710	2724	2732	rBV3	149213	326957	1.20%	0.121%
8	10.625	2745	2753	2763	rVB	214633	345698	1.27%	0.128%
9	10.718	2771	2782	2794	rVB	680595	1157348	4.25%	0.430%
10	10.818	2800	2813	2826	rBV	555658	1152555	4.23%	0.428%
11	10.889	2827	2835	2842	rBV2	275177	476292	1.75%	0.177%
12	10.950	2846	2854	2862	rBV	754404	1124131	4.13%	0.418%
13	11.005	2862	2871	2881	rVB	1506890	2582662	9.49%	0.959%
14	11.059	2882	2888	2895	rVB	285507	393763	1.45%	0.146%
15	11.124	2896	2908	2916	rBV2	1443537	2615012	9.61%	0.971%
16	11.207	2916	2934	2950	rVB6	1785819	5248727	19.28%	1.950%
17	11.291	2950	2960	2967	rBV	501145	807640	2.97%	0.300%
18	11.407	2984	2996	3014	rBV2	1191391	2704266	9.94%	1.005%
19	11.490	3014	3022	3029	rBV3	274843	447360	1.64%	0.166%
20	11.542	3029	3038	3044	rBV	1056940	1654399	6.08%	0.615%
21	11.593	3045	3054	3063	rBV6	1352581	2592017	9.52%	0.963%
22	11.654	3063	3073	3081	rBV	5304475	9527363	35.01%	3.539%
23	11.696	3081	3086	3097	rVB2	3575913	5588449	20.53%	2.076%
24	11.757	3097	3105	3111	rBV3	668863	1211873	4.45%	0.450%
25	11.812	3112	3122	3127	rBV3	578272	1102230	4.05%	0.409%
26	11.850	3127	3134	3142	rVB3	1972915	2982415	10.96%	1.108%
27	11.921	3142	3156	3169	rBV5	7089241	17795254	65.38%	6.611%
28	12.043	3187	3194	3202	rBV	7080507	9411061	34.58%	3.496%
29	12.082	3202	3206	3208	rVV2	873224	794122	2.92%	0.295%
30	12.120	3210	3218	3223	rVV3	6054515	10478741	38.50%	3.893%
31	12.165	3224	3232	3249	rVB5	11255878	22338980	82.08%	8.299%
32	12.403	3295	3306	3316	rBV6	2604935	5302741	19.48%	1.970%
33	12.490	3316	3333	3339	rBV5	2646517	7908695	29.06%	2.938%
34	12.561	3348	3355	3371	rVB4	8548020	18144853	66.67%	6.741%

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35	12.644	3371	3381	3390	rBV5	3661568	8001442	29.40%	2.973%
36	12.728	3393	3407	3416	rVV6	10274068	27217115	100.00%	10.111%
37	12.779	3417	3423	3433	rVB2	5734564	9010912	33.11%	3.348%
38	12.866	3444	3450	3457	rVV4	2743107	3709677	13.63%	1.378%
39	12.924	3458	3468	3472	rVV3	2111353	4600842	16.90%	1.709%
40	12.960	3472	3479	3493	rVB3	8406716	15209683	55.88%	5.650%
41	13.239	3552	3566	3586	rVB	7876136	18189193	66.83%	6.757%
42	13.609	3670	3681	3687	rBV2	1413666	2904965	10.67%	1.079%
43	13.660	3688	3697	3707	rVB3	6675106	11666867	42.87%	4.334%
44	13.886	3761	3767	3777	rVB2	3407470	5341430	19.63%	1.984%
45	13.992	3791	3800	3809	rVB5	1656473	2856499	10.50%	1.061%
46	14.175	3847	3857	3883	rVB8	2591665	8955192	32.90%	3.327%
47	14.291	3886	3893	3898	rBV2	585637	901205	3.31%	0.335%
48	14.329	3899	3905	3912	rVB2	1108648	1454177	5.34%	0.540%
49	14.525	3961	3966	3973	rVB4	227432	290730	1.07%	0.108%
50	14.580	3973	3983	3995	rVV2	1618756	3110496	11.43%	1.156%
51	14.644	3996	4003	4014	rVB3	547457	935989	3.44%	0.348%
52	14.847	4062	4066	4073	rVB3	280114	343515	1.26%	0.128%

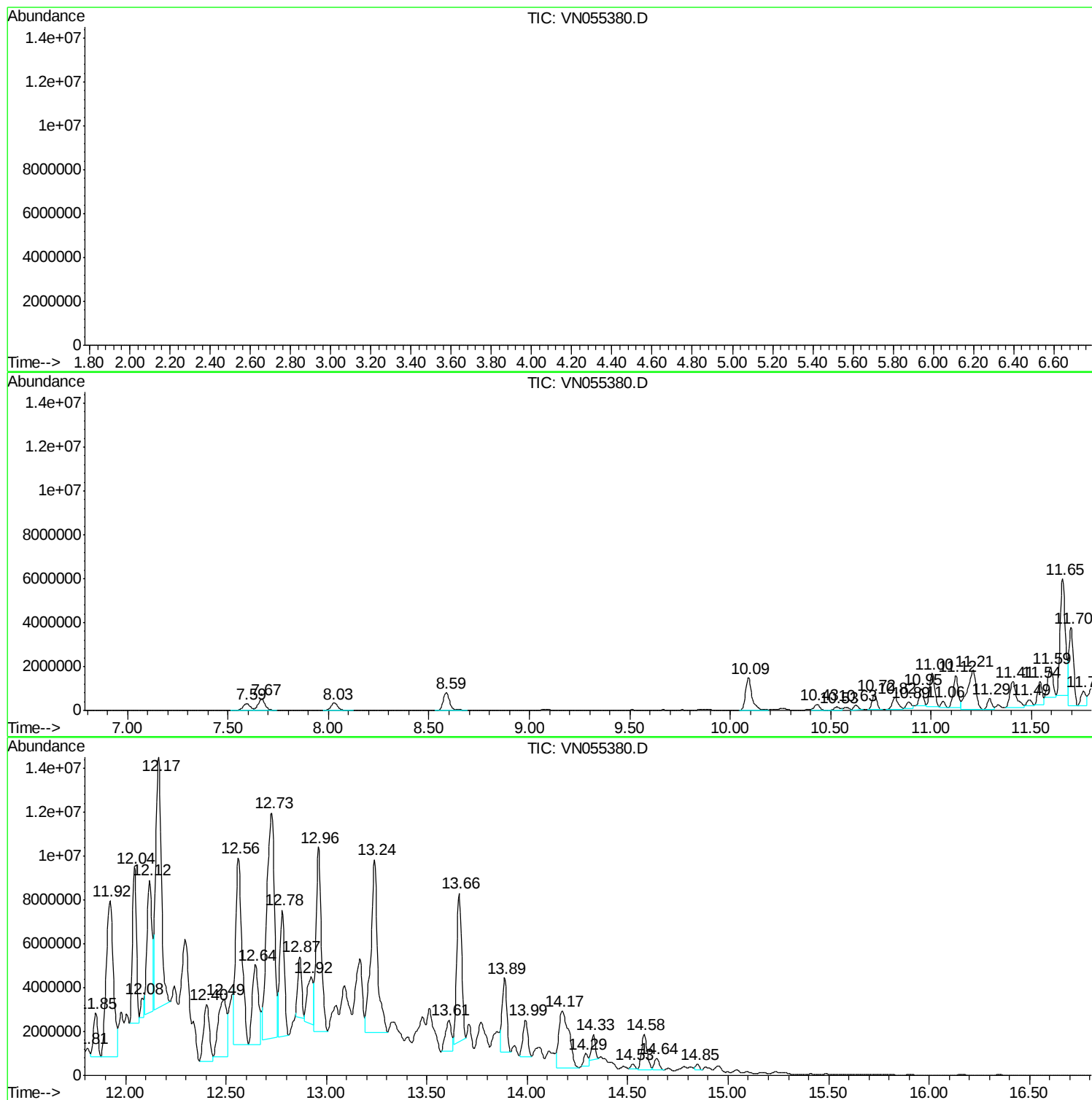
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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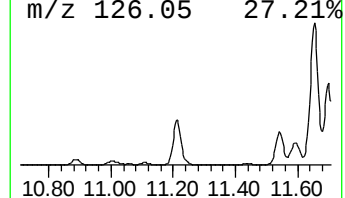
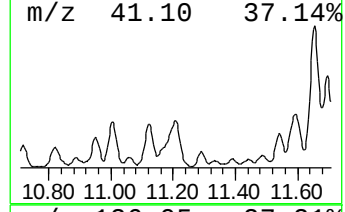
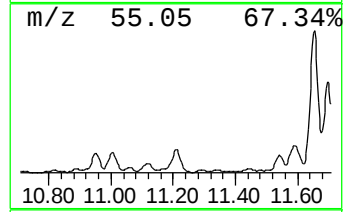
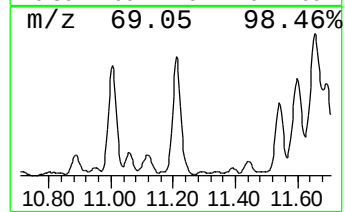
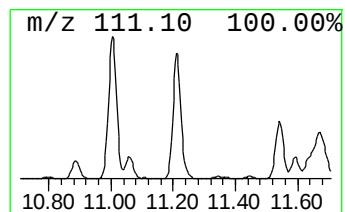
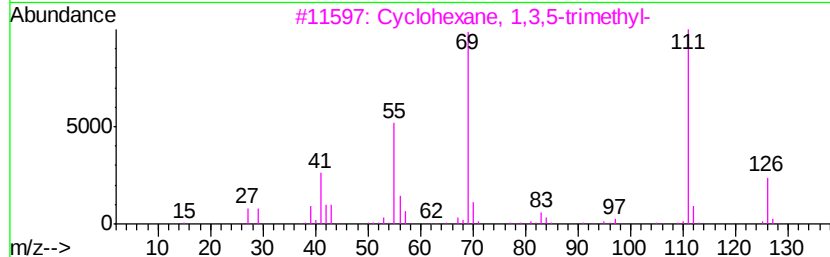
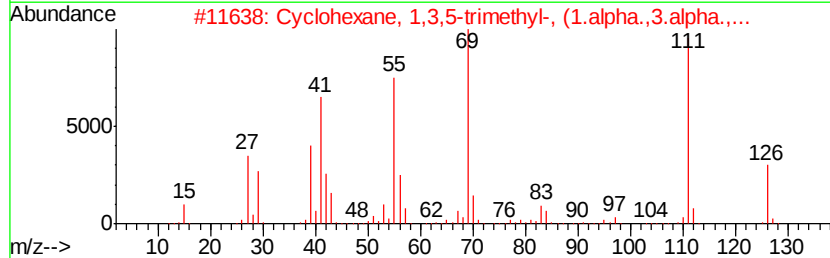
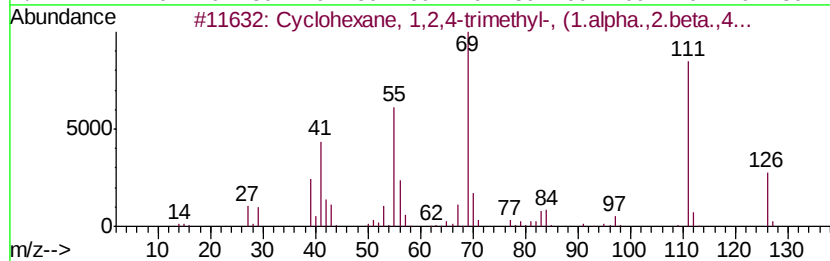
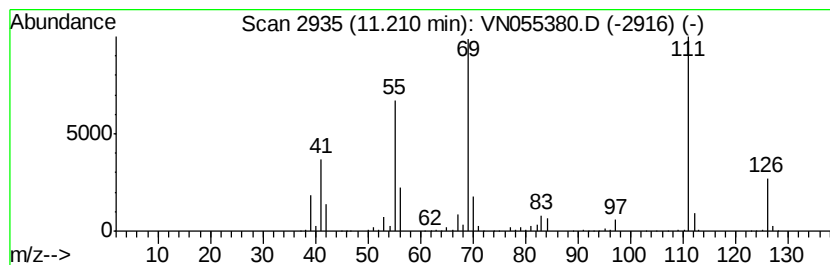
Instrument :
MSVOA_N
ClientSampleId :
EP1-SB-E3-4(17-20)

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N042919W.M
Quant Title : SW846 8260

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

Peak Number 1 Cyclohexane, 1,2,4-trimethy... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.		
11.21	97.05 ug/l	5248730	Chlorobenzene-d5	11.41		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,2,4-trimethyl-, (...	126	C9H18		007667-60-9	94
2	Cyclohexane, 1,3,5-trimethyl-, (...	126	C9H18		001795-26-2	91
3	Cyclohexane, 1,3,5-trimethyl-	126	C9H18		001839-63-0	91
4	Cyclohexane, 1,3,5-trimethyl-, (...	126	C9H18		001795-27-3	87
5	2-Pyrazoline, 1-isopropyl-5-methyl-	126	C7H14N2		026964-54-5	64



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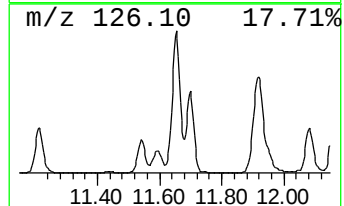
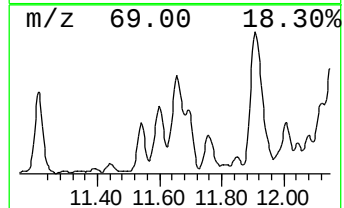
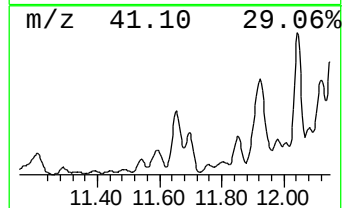
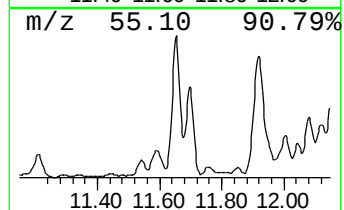
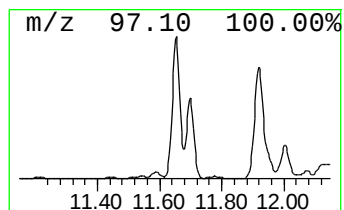
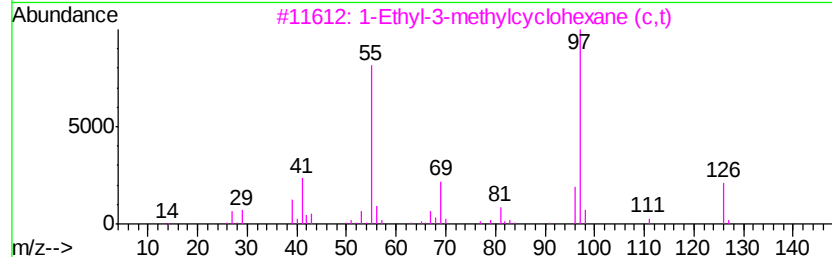
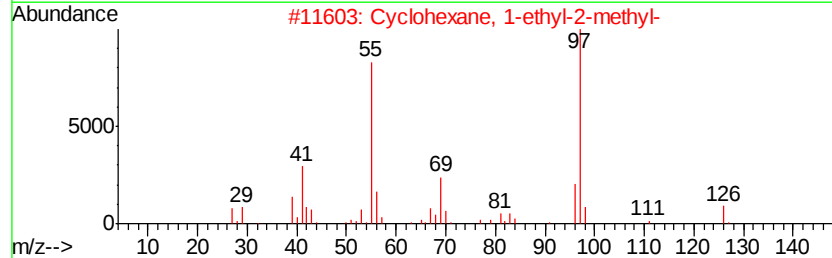
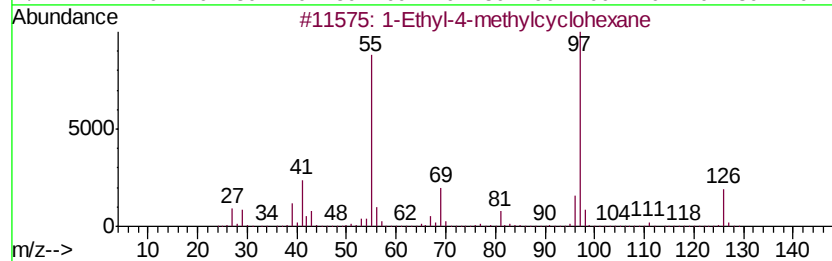
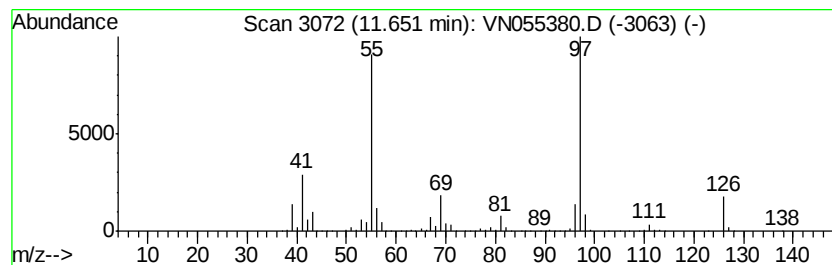
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N042919W.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 1-Ethyl-4-methylcyclohexane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.65	176.15 ug/l	9527360	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		Cyclohexane, 1-ethyl-2-methyl-	126	C9H18	003728-54-9	90
3		1-Ethyl-3-methylcyclohexane (c,t)	126	C9H18	003728-55-0	90
4		cis-1-Ethyl-3-methyl-cyclohexane	126	C9H18	019489-10-2	90
5		Cyclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-78-8	87



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MSVOA_N
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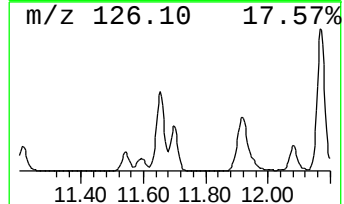
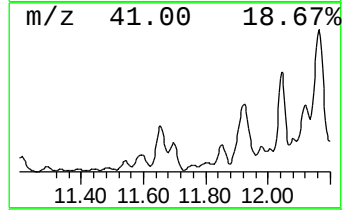
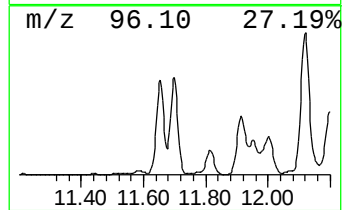
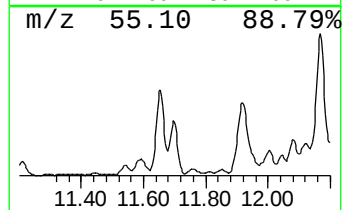
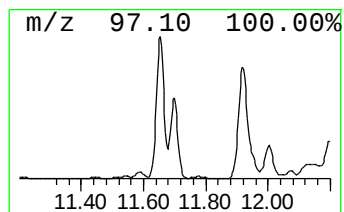
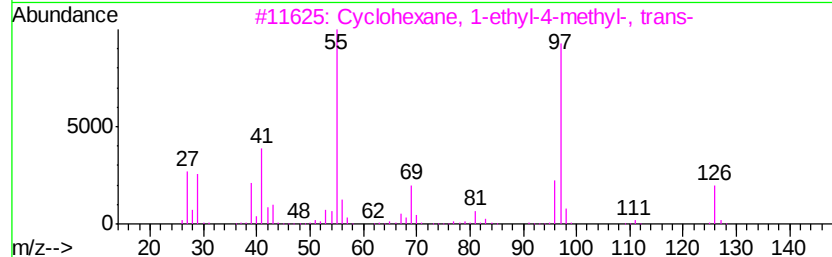
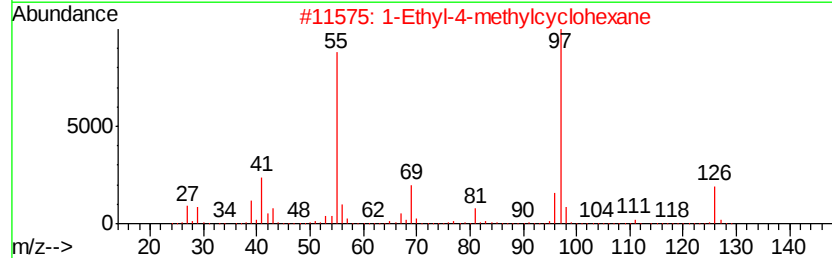
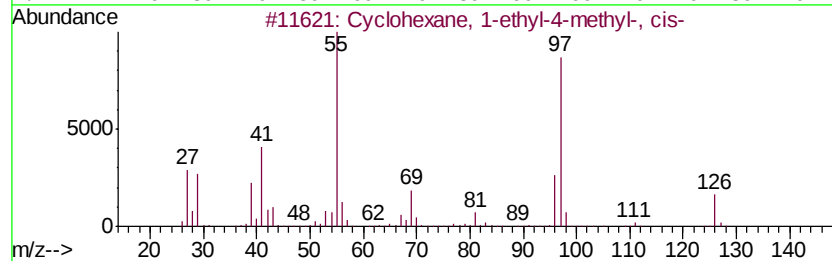
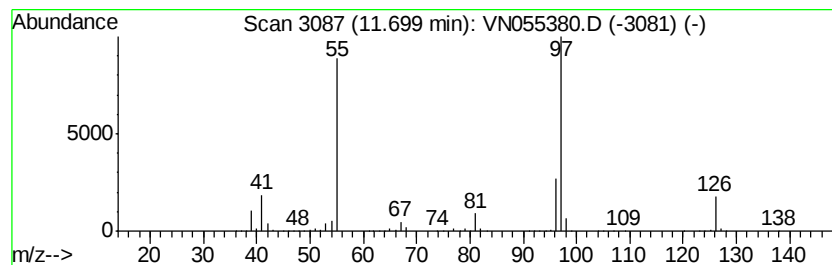
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 Cyclohexane, 1-ethyl-4-meth... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.70	103.33 ug/l	5588450	Chlorobenzene-d5	11.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	004926-78-7	90
2		1-Ethyl-4-methylcyclohexane	126	C9H18	003728-56-1	87
3		Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	006236-88-0	83
4		Cyclopentane, 1,1'-ethylidenebis-	166	C12H22	004413-21-2	72
5		Cyclohexane, 1-ethyl-1-methyl-	126	C9H18	004926-90-3	72



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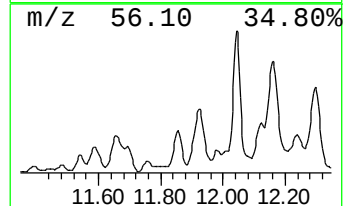
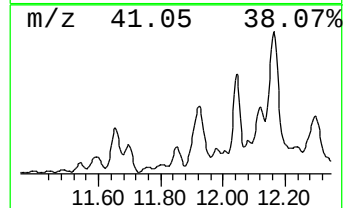
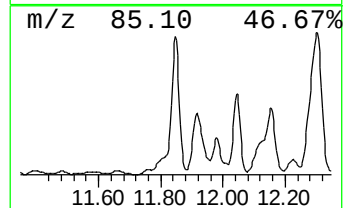
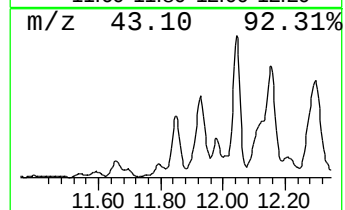
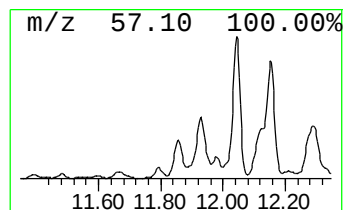
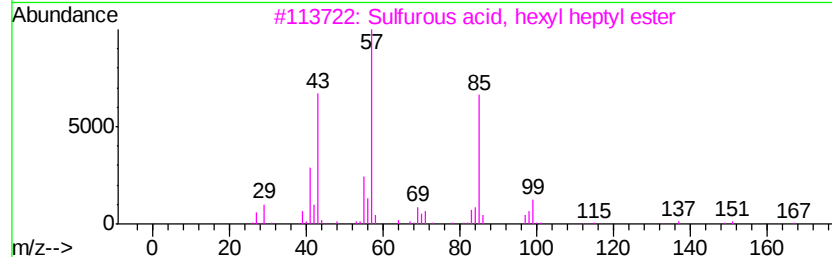
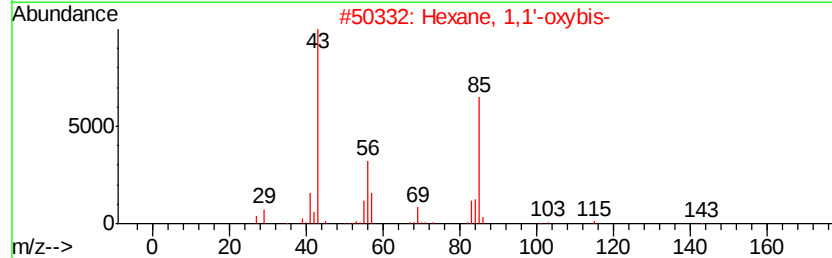
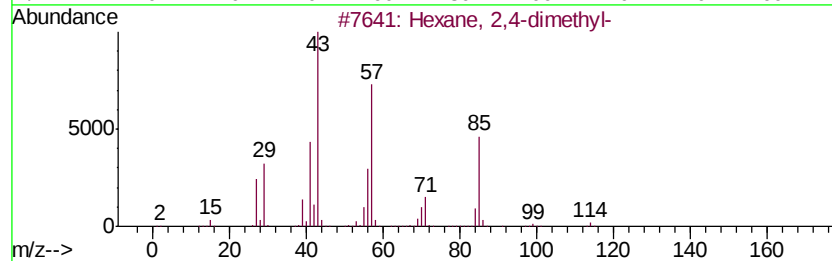
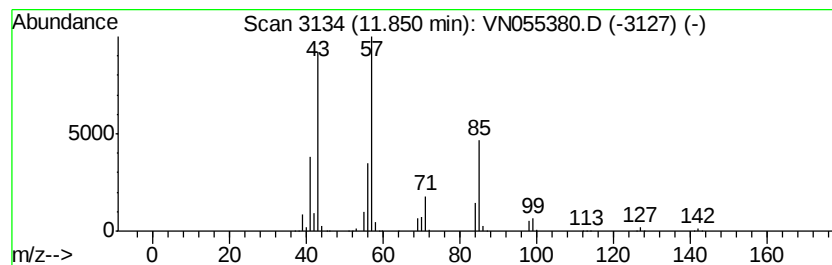
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Peak Number 4 Hexane, 2,4-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.		
11.85	55.14 ug/l	2982420	Chlorobenzene-d5	11.41		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 2,4-dimethyl-		114	C8H18	000589-43-5	72
2	Hexane, 1,1'-oxybis-		186	C12H26O	000112-58-3	59
3	Sulfurous acid, hexyl heptyl ester		264	C13H28O3S	1000309-12-9	59
4	Oxalic acid, butyl isohexyl ester		230	C12H22O4	1000309-32-7	59
5	Heptane, 2,4-dimethyl-		128	C9H20	002213-23-2	50



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ALS Vial : 6 Sample Multiplier: 1

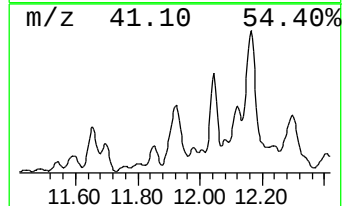
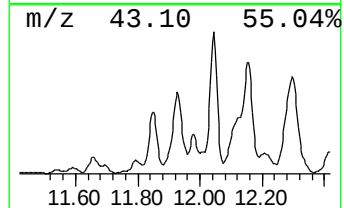
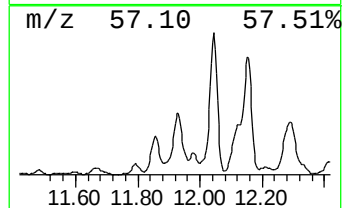
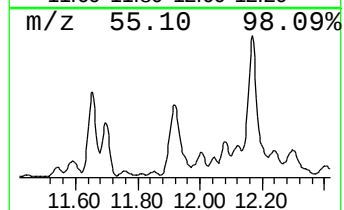
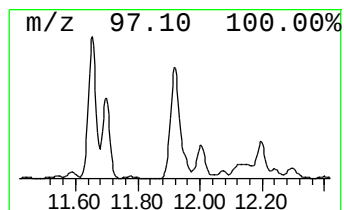
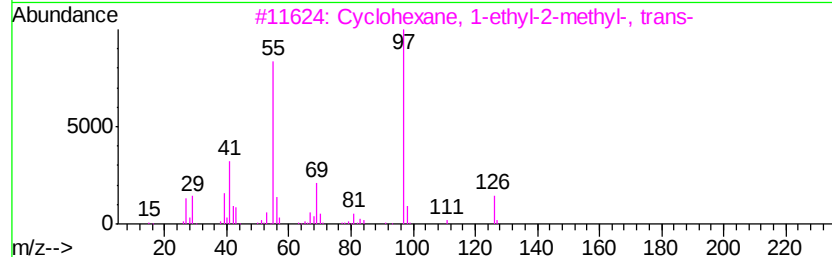
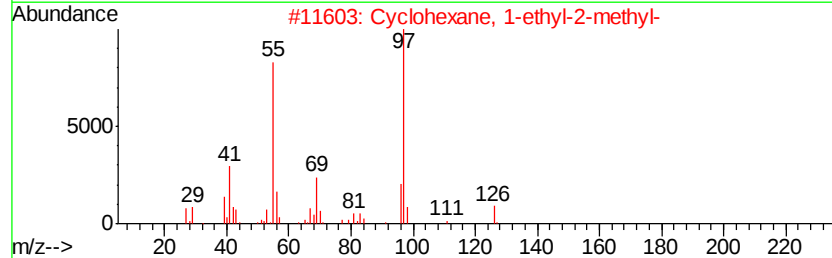
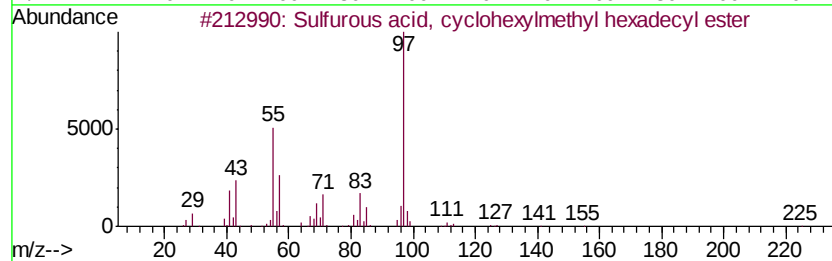
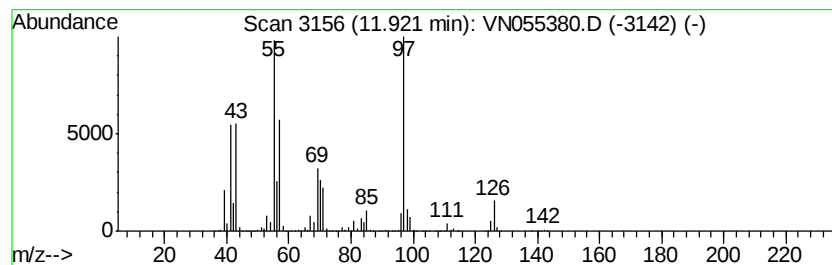
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MSVOA_N
ClientSampleId :
EP1-SB-E3-4(17-20)

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N042919W.M
Quant Title : SW846 8260

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

Peak Number 5 Sulfurous acid, cyclohexylm... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.		
11.92	329.02 ug/l	17795300	Chlorobenzene-d5	11.41		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Sulfurous acid, cyclohexylmethyl-	402	C23H46O3S	1000309-22-4	64
2		Cyclohexane, 1-ethyl-2-methyl-	126	C9H18	003728-54-9	64
3		Cyclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-78-8	58
4		Cyclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-77-7	52
5		Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	006236-88-0	50



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN050319\
Data File : VN055380.D
Acq On : 3 May 2019 11:12
Operator : JC/SP
Sample : K2658-08 10X
Misc : 5.17g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 6 Sample Multiplier: 1

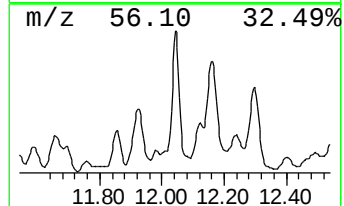
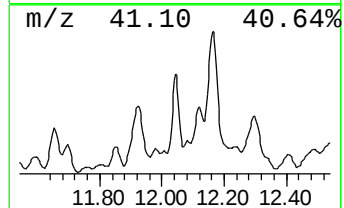
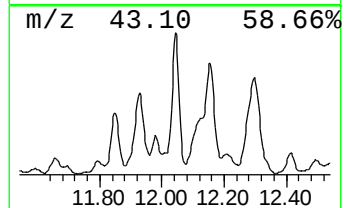
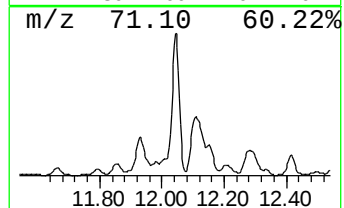
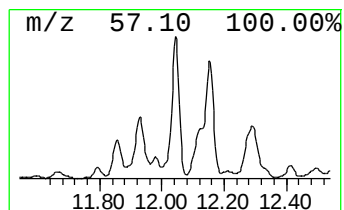
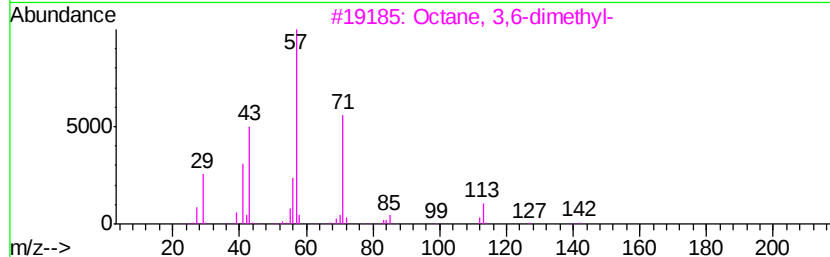
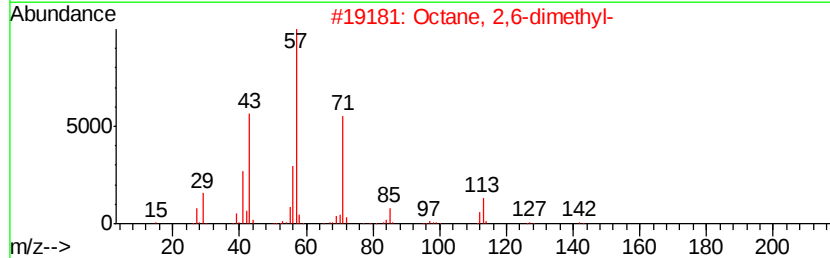
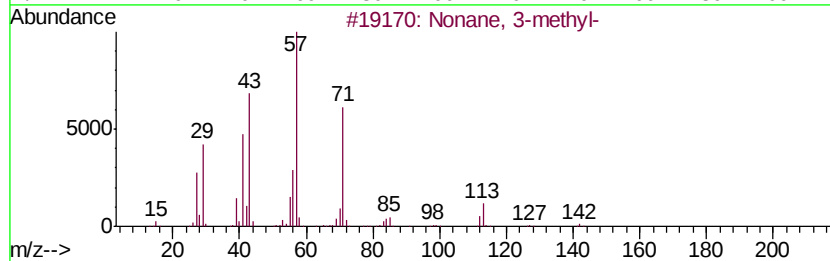
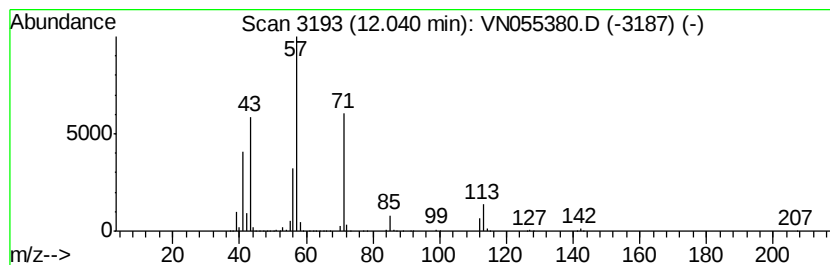
Instrument :
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ClientSampleId :
EP1-SB-E3-4(17-20)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N042919W.M
Quant Title : SW846 8260

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

Peak Number 6 Nonane, 3-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.		
12.04	174.00 ug/l	9411060	Chlorobenzene-d5	11.41		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Nonane, 3-methyl-	142	C10H22	005911-04-6	91
2		Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	87
3		Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	87
4		Decane, 2,6,7-trimethyl-	184	C13H28	062108-25-2	64
5		Sulfurous acid, 2-ethylhexyl hex...	418	C24H50O3S	1000309-19-9	53



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN050319\
Data File : VN055380.D
Acq On : 3 May 2019 11:12
Operator : JC/SP
Sample : K2658-08 10X
Misc : 5.17g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 6 Sample Multiplier: 1

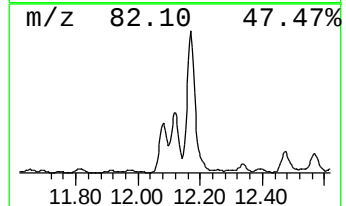
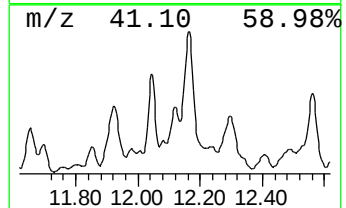
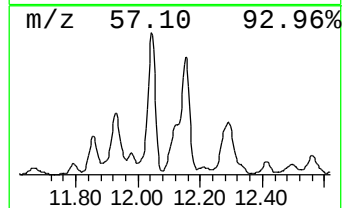
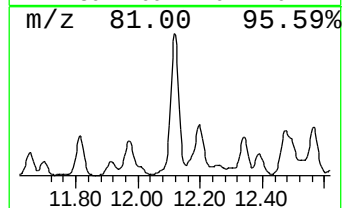
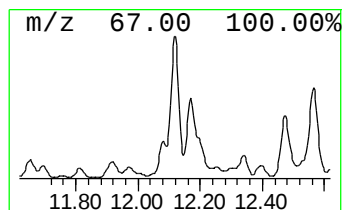
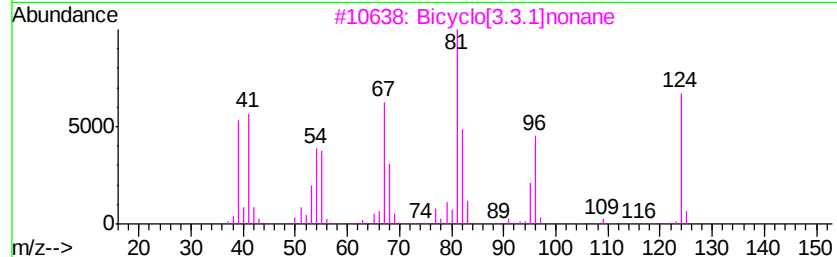
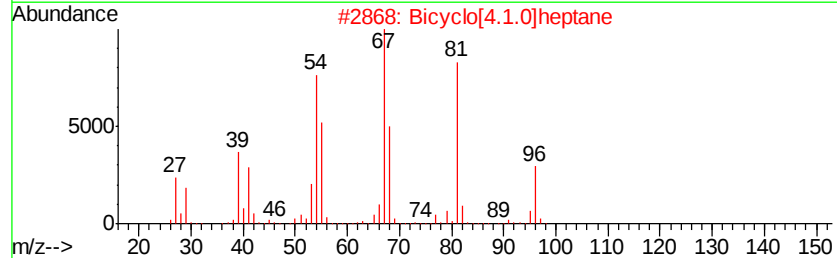
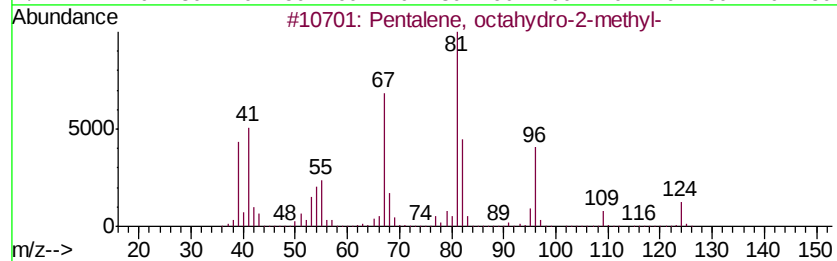
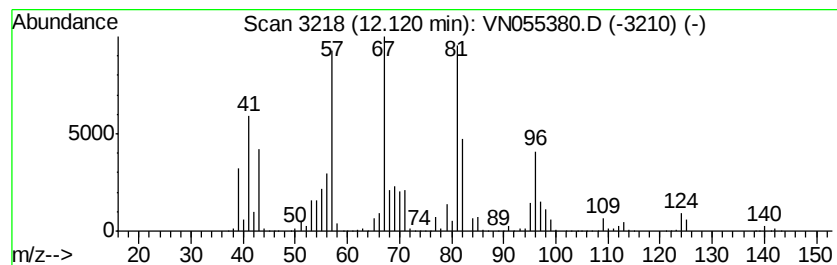
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ClientSampleId :
EP1-SB-E3-4(17-20)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N042919W.M
Quant Title : SW846 8260

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

Peak Number 7 Pentalene, octahydro-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.		
12.12	193.75 ug/l	10478700	Chlorobenzene-d5	11.41		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentalene, octahydro-2-methyl-	124	C9H16	003868-64-2	91
2		Bicyclo[4.1.0]heptane	96	C7H12	000286-08-8	58
3		Bicyclo[3.3.1]nonane	124	C9H16	000280-65-9	58
4		1H-Indene, octahydro-, trans-	124	C9H16	003296-50-2	53
5		Cyclohexene, 1-methyl-	96	C7H12	000591-49-1	46



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_N\DATA\VN050319\
Data File : VN055380.D
Acq On : 3 May 2019 11:12
Operator : JC/SP
Sample : K2658-08 10X
Misc : 5.17g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
EP1-SB-E3-4(17-20)

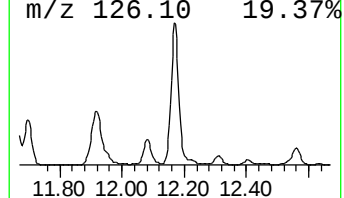
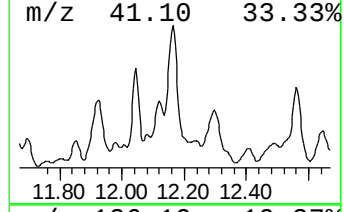
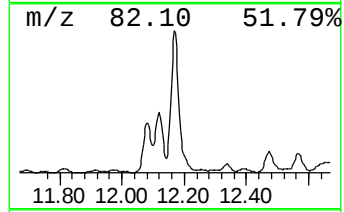
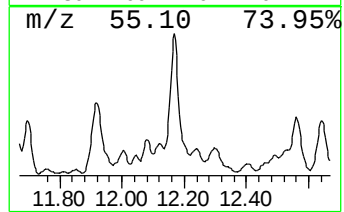
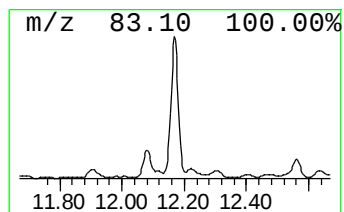
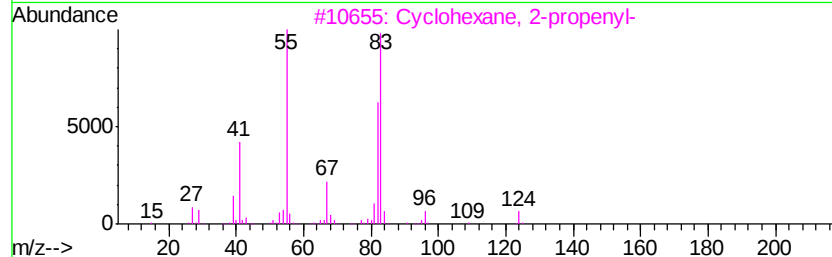
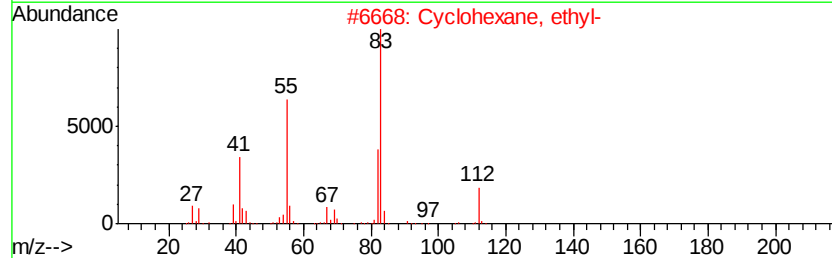
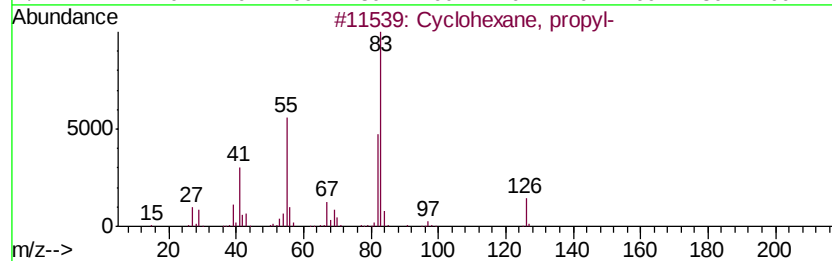
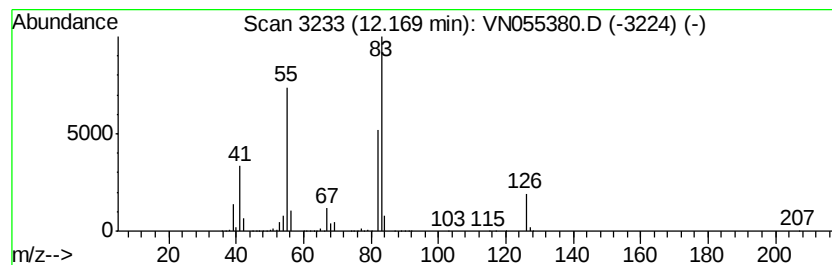
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Quant Title : SW846 8260

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

Peak Number 8 Cyclohexane, propyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.17	413.03 ug/l	22339000	Chlorobenzene-d5	11.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, propyl-	126	C9H18	001678-92-8	90
2		Cyclohexane, ethyl-	112	C8H16	001678-91-7	59
3		Cyclohexane, 2-propenyl-	124	C9H16	002114-42-3	59
4		Ethanone, 1-(1-methylcyclopentyl)-	126	C8H14O	013388-93-7	59
5		Oxalic acid, cyclohexyl nonyl ester	298	C17H30O4	1000309-31-1	53



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_N\DATA\VN050319\
Data File : VN055380.D
Acq On : 3 May 2019 11:12
Operator : JC/SP
Sample : K2658-08 10X
Misc : 5.17g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
EP1-SB-E3-4(17-20)

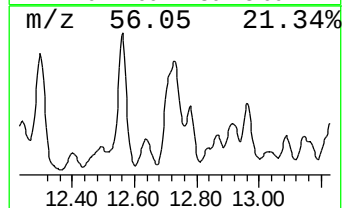
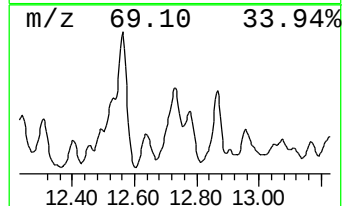
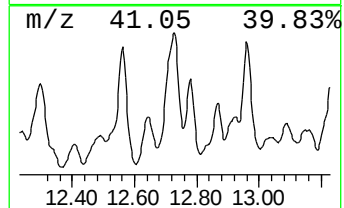
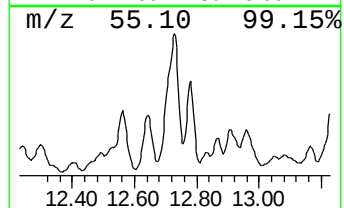
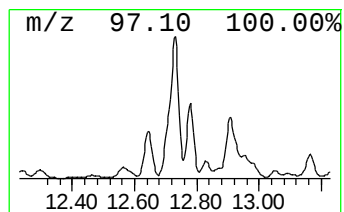
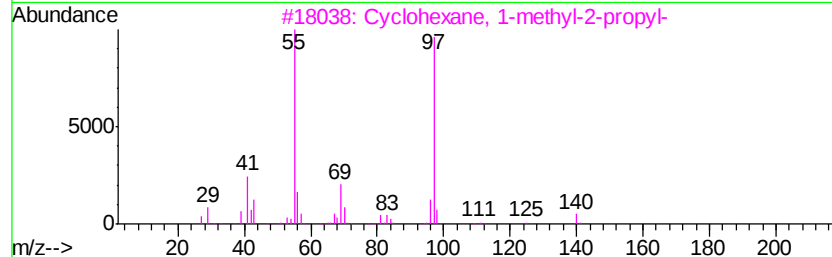
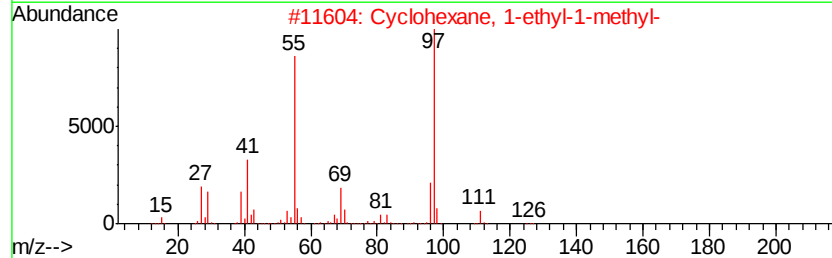
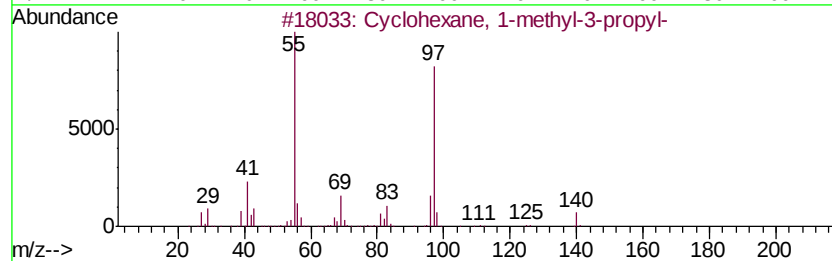
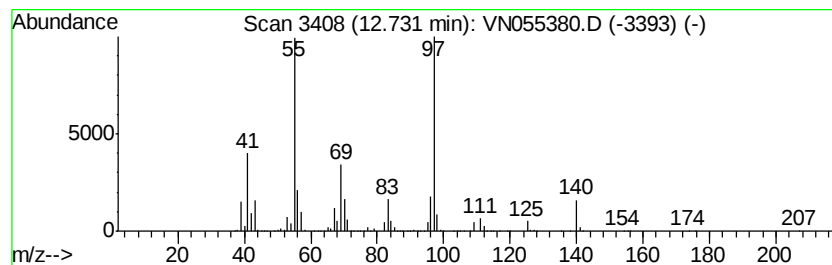
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Quant Title : SW846 8260

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

Peak Number 9 Cyclohexane, 1-methyl-3-pro... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.73	74.82 ug/l	27217100	1,4-Dichlorobenzene-d4	13.34

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, 1-methyl-3-propyl-	140	C10H20	004291-80-9	72
2		Cyclohexane, 1-ethyl-1-methyl-	126	C9H18	004926-90-3	64
3		Cyclohexane, 1-methyl-2-propyl-	140	C10H20	004291-79-6	64
4		1-Ethyl-4-methylcyclohexane	126	C9H18	003728-56-1	64
5		Cyclohexane, 1-methyl-4-(1-methy...	140	C10H20	006069-98-3	58



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_N\DATA\VN050319\
Data File : VN055380.D
Acq On : 3 May 2019 11:12
Operator : JC/SP
Sample : K2658-08 10X
Misc : 5.17g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 6 Sample Multiplier: 1

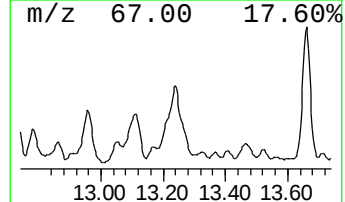
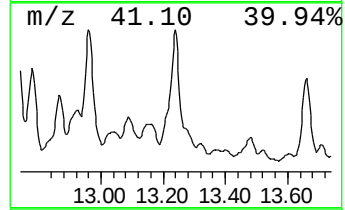
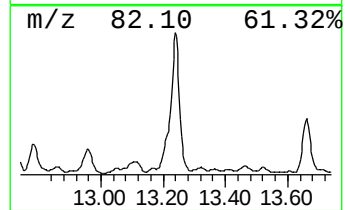
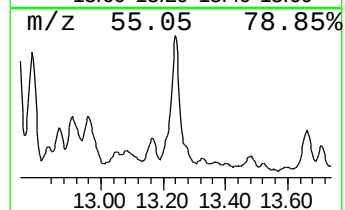
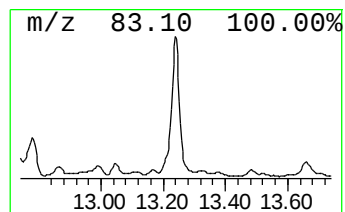
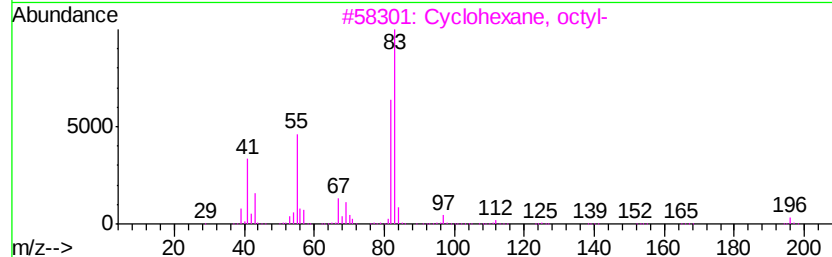
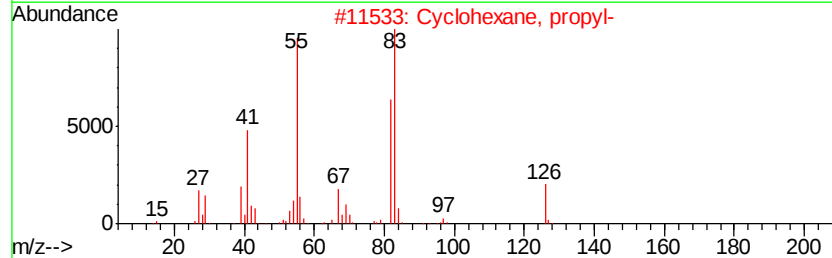
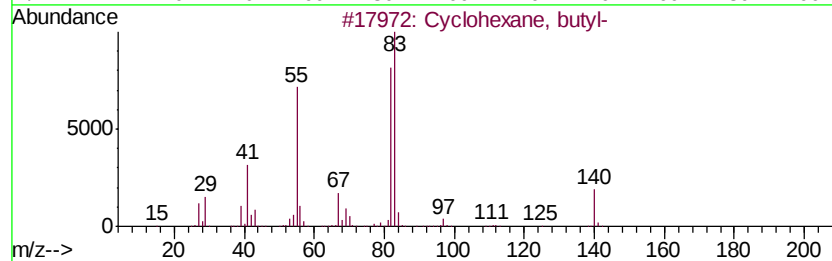
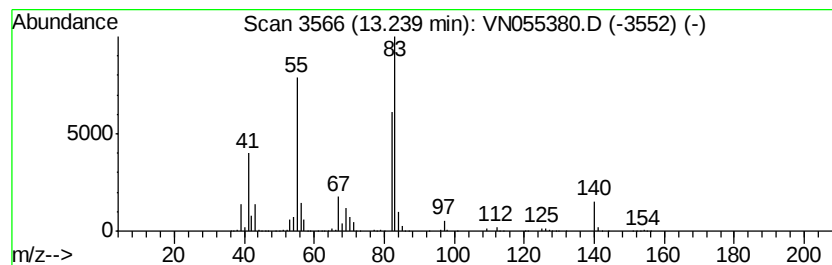
Instrument :
MSVOA_N
ClientSampleId :
EP1-SB-E3-4(17-20)

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N042919W.M
Quant Title : SW846 8260

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

Peak Number 10 Cyclohexane, butyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.24	50.00 ug/l	18189200	1,4-Dichlorobenzene-d4	13.34
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Cyclohexane, butyl-	140 C10H20	001678-93-9 97
2		Cyclohexane, propyl-	126 C9H18	001678-92-8 87
3		Cyclohexane, octyl-	196 C14H28	001795-15-9 80
4		Cyclohexane, pentyl-	154 C11H22	004292-92-6 70
5		Oxalic acid, cyclohexyl dodecyl ...	340 C20H36O4	1000309-31-4 59



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN050319\
Data File : VN055380.D
Acq On : 3 May 2019 11:12
Operator : JC/SP
Sample : K2658-08 10X
Misc : 5.17g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
EP1-SB-E3-4(17-20)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N042919W.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, 1,2,...	11.21	97.0	ug/l	5248730	3	11.41	2704270	50.0
1-Ethyl-4-methylc...	11.65	176.2	ug/l	9527360	3	11.41	2704270	50.0
Cyclohexane, 1-et...	11.70	103.3	ug/l	5588450	3	11.41	2704270	50.0
Hexane, 2,4-dimet...	11.85	55.1	ug/l	2982420	3	11.41	2704270	50.0
Sulfurous acid, c...	11.92	329.0	ug/l	17795300	3	11.41	2704270	50.0
Nonane, 3-methyl-	12.04	174.0	ug/l	9411060	3	11.41	2704270	50.0
Pentalene, octahy...	12.12	193.8	ug/l	10478700	3	11.41	2704270	50.0
Cyclohexane, propyl-	12.17	413.0	ug/l	22339000	3	11.41	2704270	50.0
Cyclohexane, 1-me...	12.73	74.8	ug/l	27217100	4	13.34	18189200	50.0
Cyclohexane, butyl-	13.24	50.0	ug/l	18189200	4	13.34	18189200	50.0