

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN032219\
 Data File : VN054590.D
 Acq On : 23 Mar 2019 6:55
 Operator : JC/SP
 Sample : K2045-16
 Misc : 5.53g/5mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 47 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 WP022SB436-190320-(24-26)

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	2.513	200	230	232	rBV10	48297	150629	2.68%	0.349%
2	2.558	236	244	263	rVB3	90966	175146	3.11%	0.406%
3	7.590	1787	1809	1819	rBV	348877	867377	15.42%	2.008%
4	7.661	1819	1831	1849	rVB	640777	1530229	27.21%	3.543%
5	8.024	1927	1944	1968	rVB2	417552	974619	17.33%	2.257%
6	8.583	2103	2118	2146	rBV	982697	2096984	37.29%	4.856%
7	9.075	2259	2271	2284	rBV4	50022	100904	1.79%	0.234%
8	9.651	2440	2450	2462	rBV2	29955	58826	1.05%	0.136%
9	10.088	2573	2586	2618	rBV	1486202	2966888	52.75%	6.870%
10	10.718	2774	2782	2794	rVB4	39597	63794	1.13%	0.148%
11	10.818	2805	2813	2826	rBV	36069	78935	1.40%	0.183%
12	11.001	2864	2870	2881	rVB4	54471	94237	1.68%	0.218%
13	11.297	2955	2962	2981	rVB	103919	223633	3.98%	0.518%
14	11.410	2984	2997	3002	rBV	1425101	2833696	50.38%	6.561%
15	11.593	3046	3054	3063	rBV5	54359	100671	1.79%	0.233%
16	11.654	3065	3073	3081	rBV4	161933	285049	5.07%	0.660%
17	11.850	3127	3134	3143	rBV4	161751	255511	4.54%	0.592%
18	11.924	3144	3157	3168	rBV6	441582	977608	17.38%	2.264%
19	11.975	3170	3173	3179	rVB2	78238	87015	1.55%	0.201%
20	12.043	3186	3194	3203	rVB	749552	1085316	19.30%	2.513%
21	12.117	3208	3217	3222	rVV2	354417	611972	10.88%	1.417%
22	12.156	3223	3229	3240	rVB5	520681	943352	16.77%	2.184%
23	12.294	3260	3272	3280	rBV9	376569	991715	17.63%	2.296%
24	12.403	3296	3306	3315	rBV	1023756	1777073	31.60%	4.115%
25	12.561	3349	3355	3369	rVB4	592278	1149149	20.43%	2.661%
26	12.644	3371	3381	3391	rBV7	227344	534985	9.51%	1.239%
27	12.728	3394	3407	3416	rBV7	655752	1576253	28.03%	3.650%
28	12.869	3444	3451	3458	rBV3	314207	491114	8.73%	1.137%
29	12.959	3473	3479	3492	rVB	1263766	2021621	35.95%	4.681%
30	13.088	3512	3519	3528	rBV	413521	666688	11.85%	1.544%
31	13.143	3530	3536	3550	rVB6	432378	968482	17.22%	2.243%
32	13.239	3552	3566	3572	rBV5	744549	1551728	27.59%	3.593%
33	13.281	3573	3579	3587	rVB2	888055	1286041	22.87%	2.978%
34	13.358	3592	3603	3618	rVB2	2380881	5624112	100.00%	13.023%

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Integration Parameters: RTEINT.P

Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
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Stop Thrs : 0 Peak Location: TOP

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Peak separation: 5

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35	13.657	3686	3696	3707	rBV4	1686461	3323658	59.10%	7.696%
36	13.991	3793	3800	3809	rBV3	332608	556280	9.89%	1.288%
37	14.178	3847	3858	3883	rVB10	854263	2584801	45.96%	5.985%
38	14.297	3888	3895	3900	rVV2	282688	445477	7.92%	1.032%
39	14.329	3901	3905	3914	rVB3	393751	538702	9.58%	1.247%
40	14.522	3961	3965	3974	rVB3	190762	247384	4.40%	0.573%
41	14.638	3996	4001	4013	rVB6	186541	289502	5.15%	0.670%

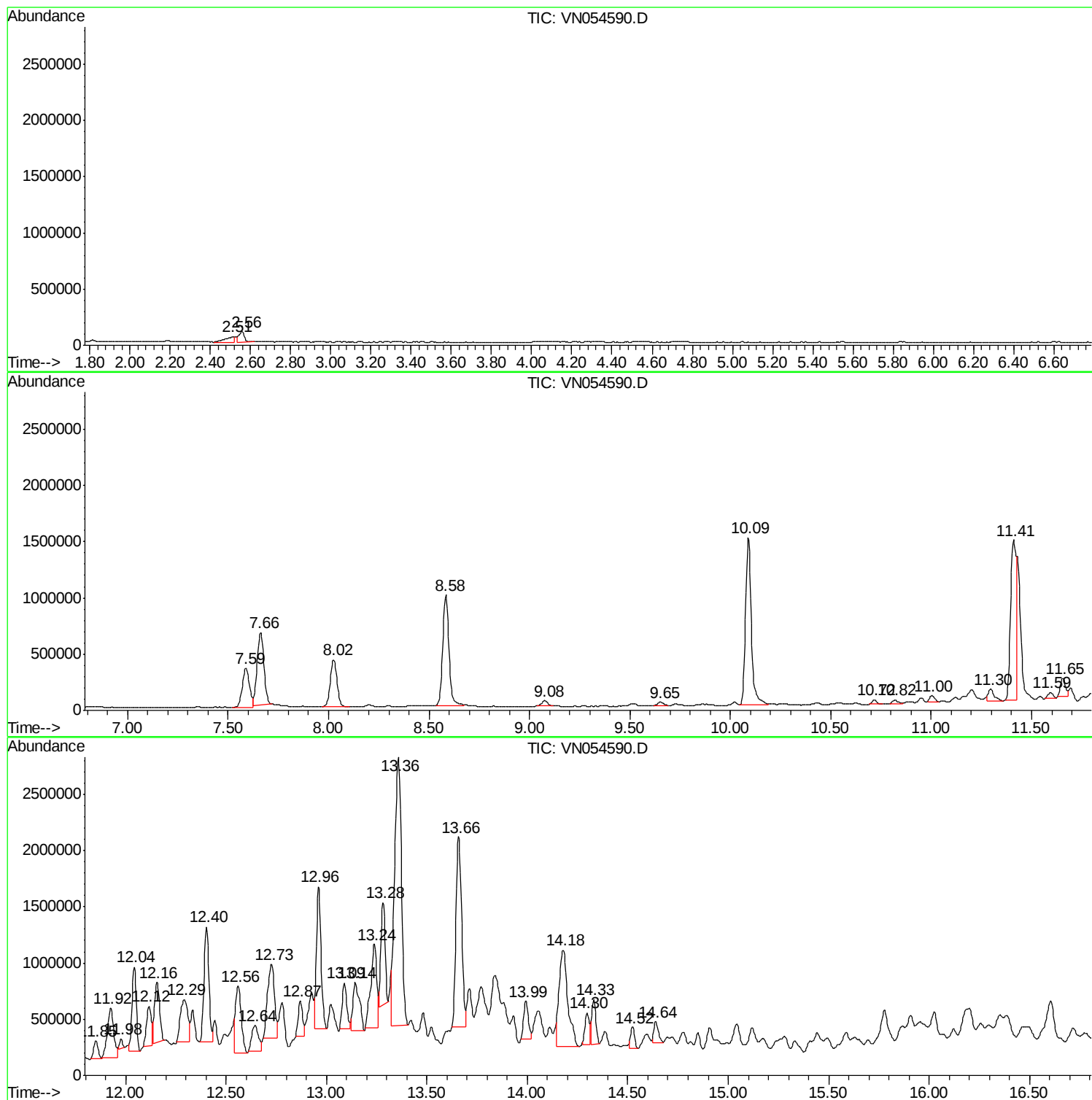
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N032019W.M
Quant Title : SW846 8260

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



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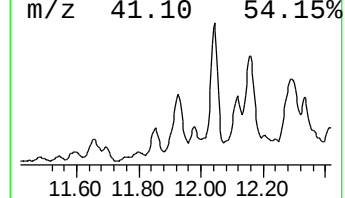
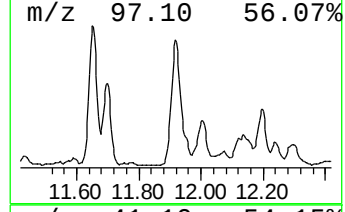
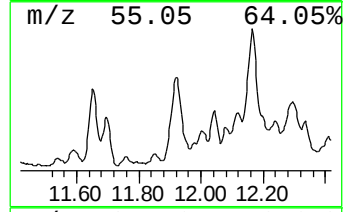
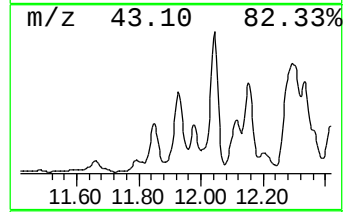
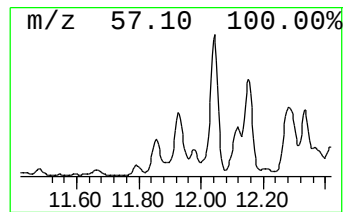
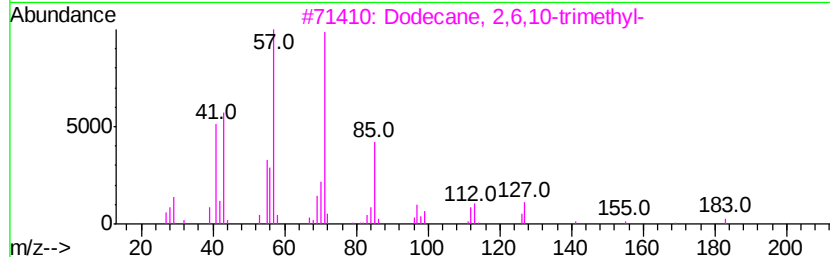
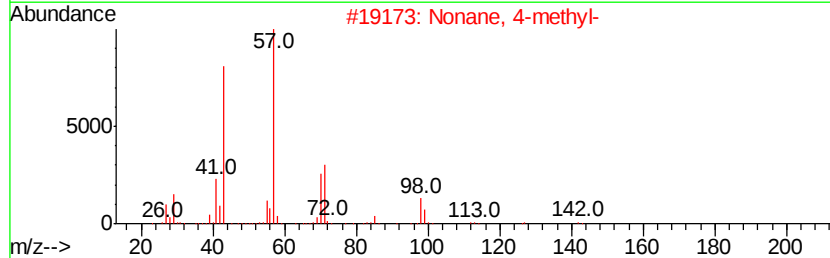
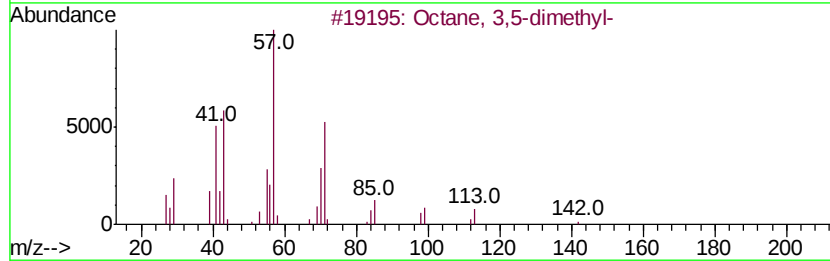
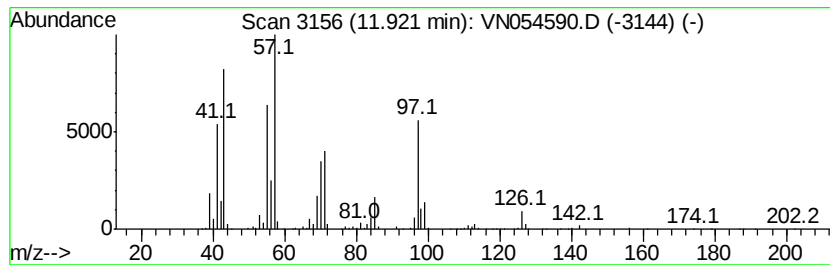
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N032019W.M
Quant Title : SW846 8260

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

Peak Number 2 unknown11.92 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	17.25 ug/l	977608	Chlorobenzene-d5	11.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	49
2		Nonane, 4-methyl-	142	C10H22	017301-94-9	46
3		Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	43
4		Octane, 2,5-dimethyl-	142	C10H22	015869-89-3	43
5		Heptane, 3-ethyl-2-methyl-	142	C10H22	014676-29-0	38



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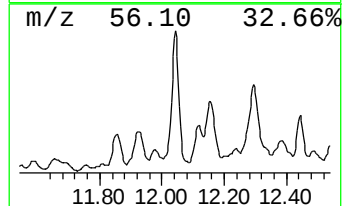
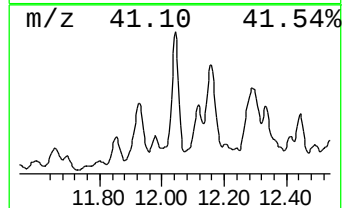
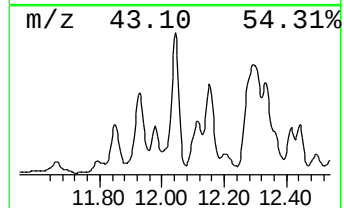
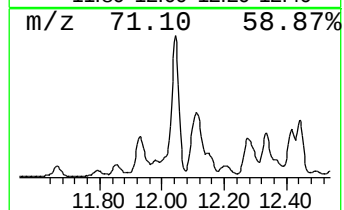
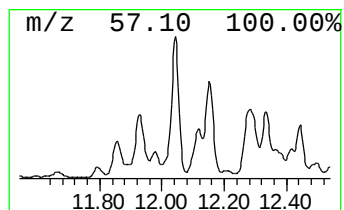
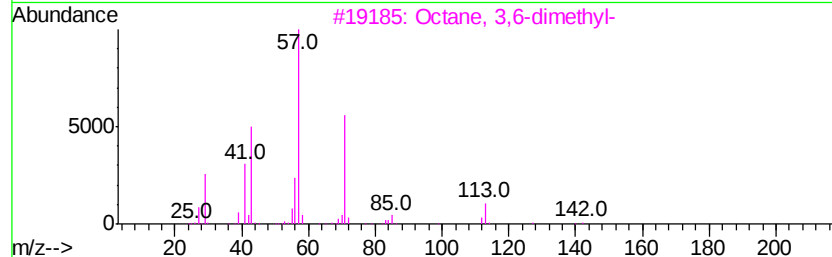
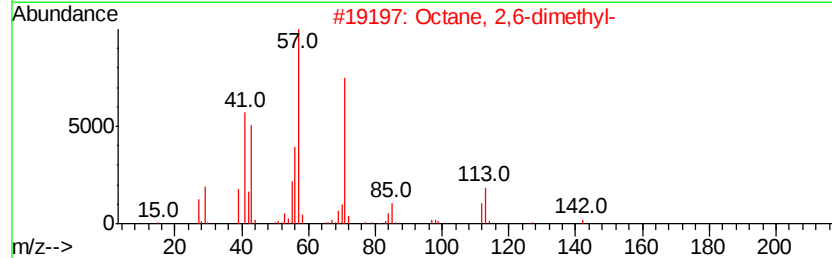
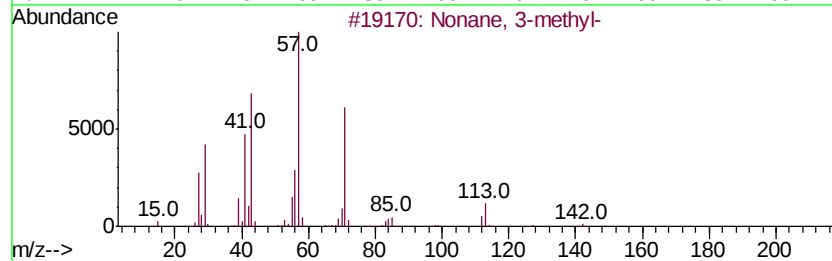
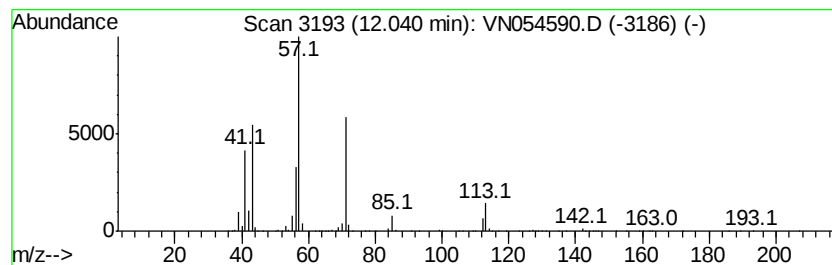
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TIC Integration Parameters: LSCINT.P

Peak Number 3 Nonane, 3-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.		
12.04	19.15 ug/l	1085320	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	86
4		Undecane, 6,6-dimethyl-	184	C13H28	017312-76-4	59
5		Nonane, 4-methyl-5-propyl-	184	C13H28	062185-55-1	59



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Misc : 5.53uL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 47 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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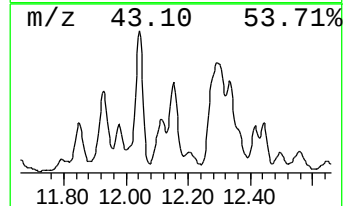
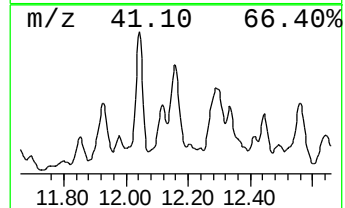
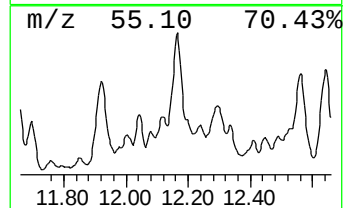
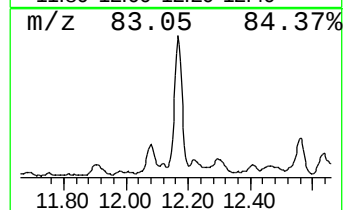
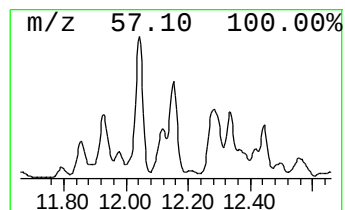
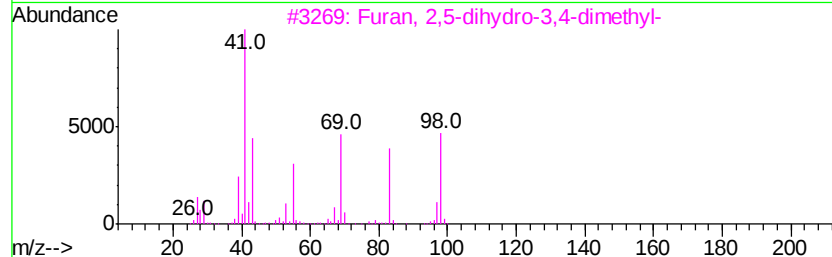
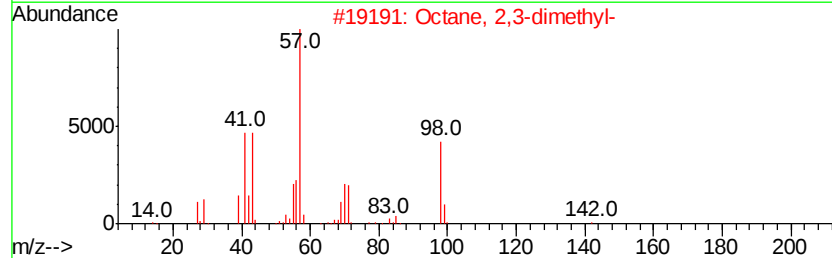
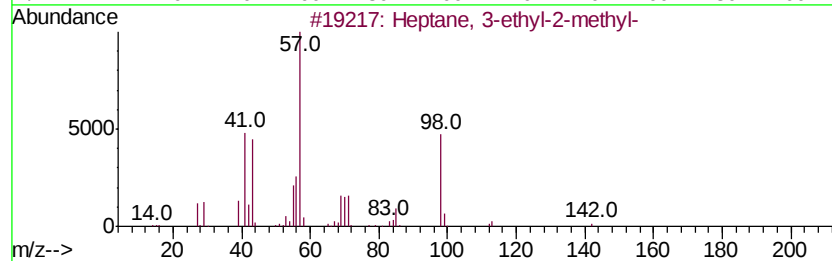
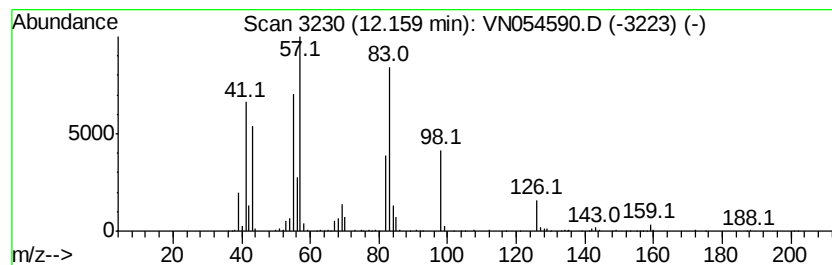
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Quant Title : SW846 8260

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

Peak Number 5 unknown12.16 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.16	16.65 ug/l	943352	Chlorobenzene-d5	11.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptane, 3-ethyl-2-methyl-	142	C10H22	014676-29-0	46
2		Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	43
3		Furan, 2,5-dihydro-3,4-dimethyl-	98	C6H10O	053720-72-2	38
4		3-Trifluoroacetoxy-6-ethyldecane	282	C14H25F3O2	116436-59-0	38
5		Heptane, 4-propyl-	142	C10H22	003178-29-8	25



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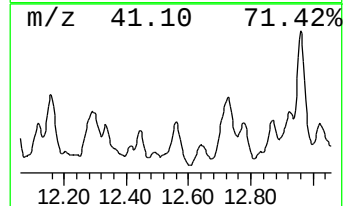
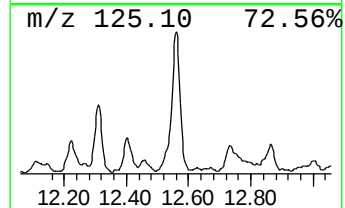
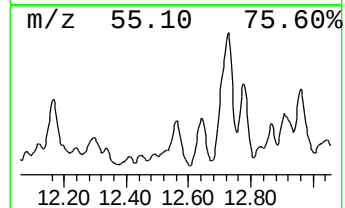
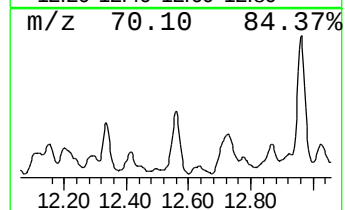
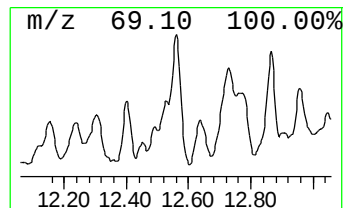
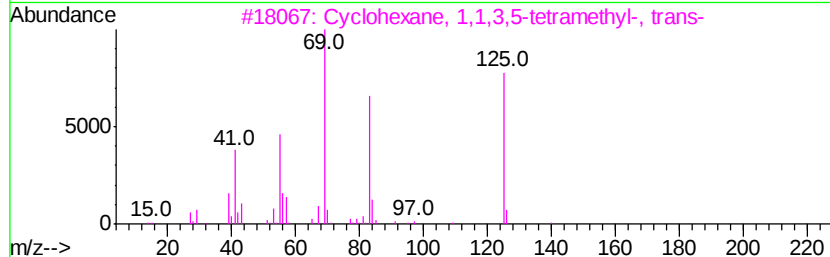
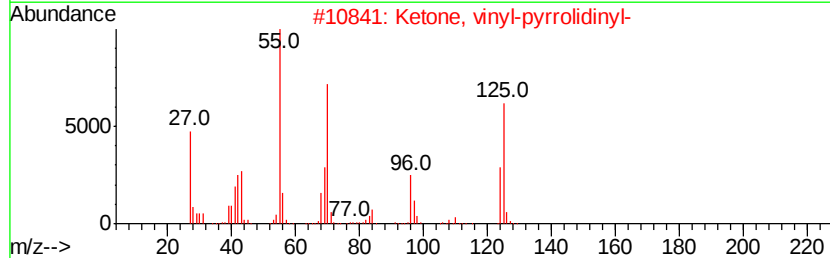
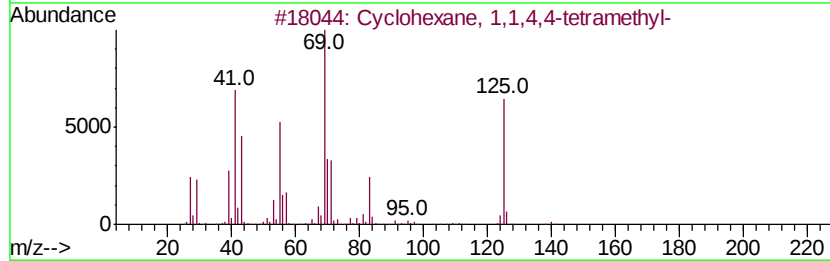
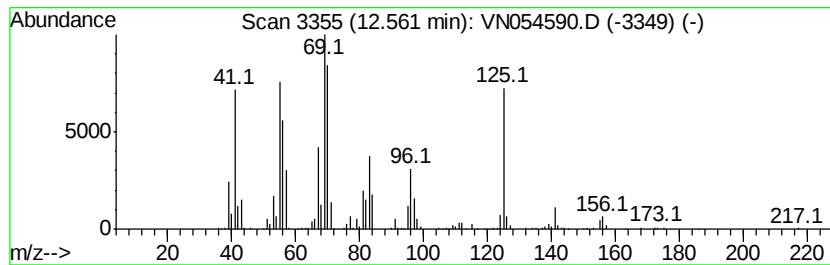
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown12.56 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.56	10.22 ug/l	1149150	1,4-Dichlorobenzene-d4	13.34

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, 1,1,4,4-tetramethyl-	140	C10H20	002223-52-1	38
2		Ketone, vinyl-pyrrolidinyl-	125	C7H11NO	042104-70-1	38
3		Cyclohexane, 1,1,3,5-tetramethyl...	140	C10H20	050876-31-8	38
4		Trifluoroacetic acid, heptyl ester	212	C9H15F3O2	002710-89-6	38
5		3-Amino-1-azabicyclo[2.2.2]octane	126	C7H14N2	006238-14-8	35



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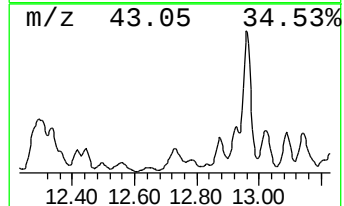
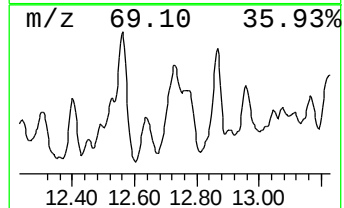
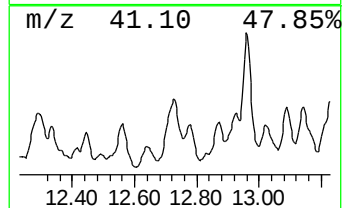
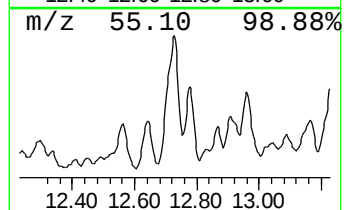
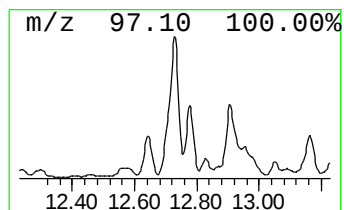
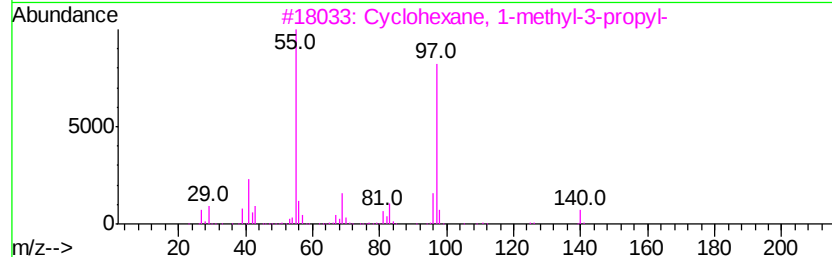
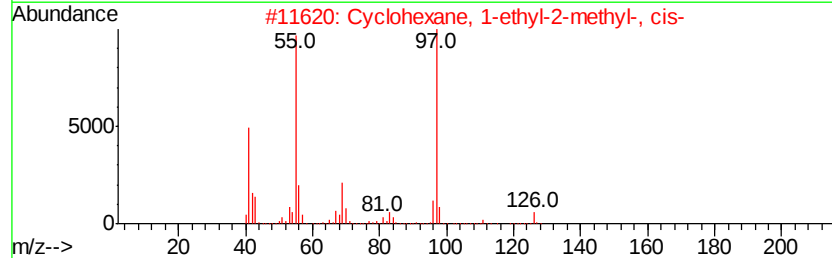
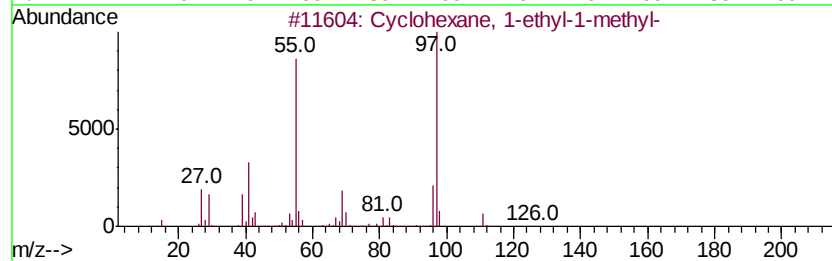
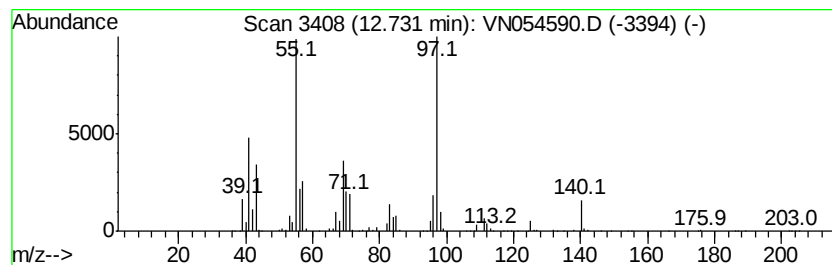
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Quant Title : SW846 8260

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

Peak Number 7 Cyclohexane, 1-ethyl-1-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.73	14.01 ug/l	1576250	1,4-Dichlorobenzene-d4	13.34

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, 1-ethyl-1-methyl-	126	C9H18	004926-90-3	64
2		Cyclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-77-7	64
3		Cyclohexane, 1-methyl-3-propyl-	140	C10H20	004291-80-9	64
4		Cyclohexane, 1,1-dimethyl-	112	C8H16	000590-66-9	58
5		Cyclohexane, 1-methyl-4-(1-methyl-...	140	C10H20	006069-98-3	52



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_N\DATA\VN032219\
Data File : VN054590.D
Acq On : 23 Mar 2019 6:55
Operator : JC/SP
Sample : K2045-16
Misc : 5.53u/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 47 Sample Multiplier: 1

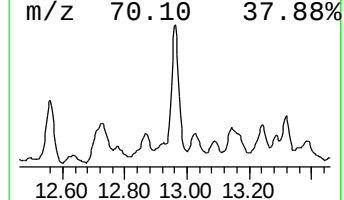
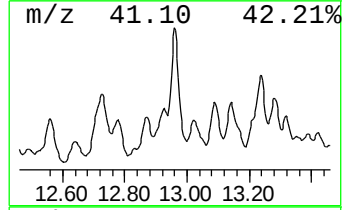
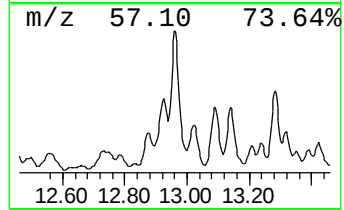
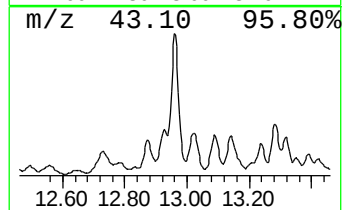
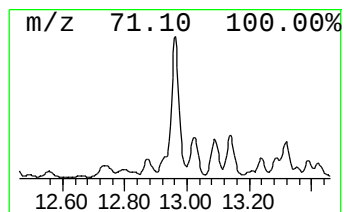
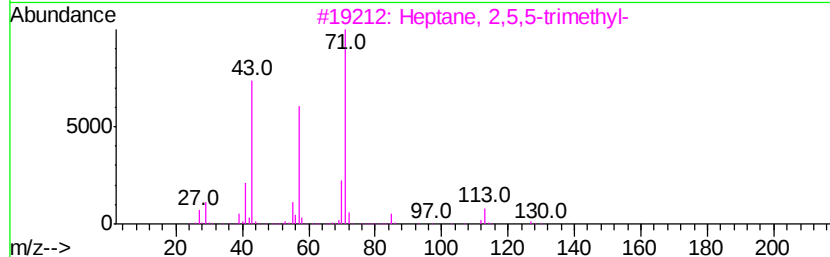
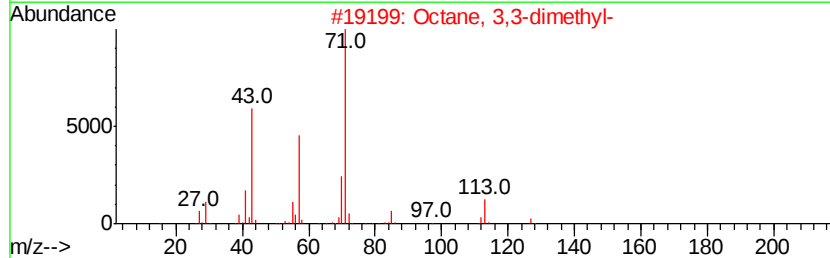
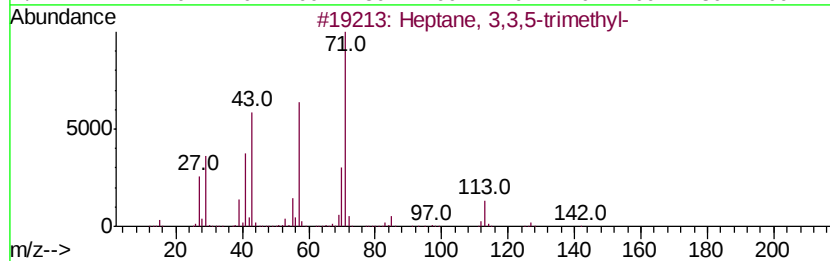
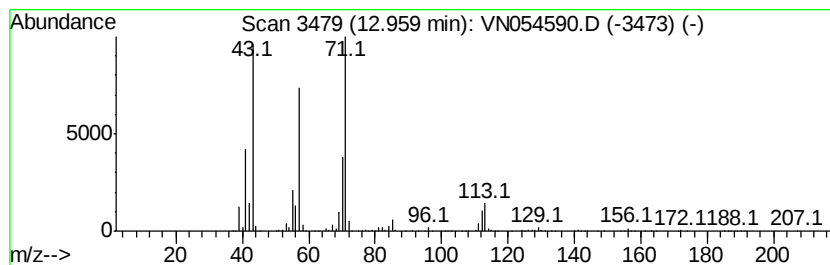
Instrument :
MSVOA_N
ClientSampleId :
WP022SB436-190320-(24-26)

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N032019W.M
Quant Title : SW846 8260

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

Peak Number 8 Heptane, 3,3,5-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.96	17.97 ug/l	2021620	1,4-Dichlorobenzene-d4	13.34
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Heptane, 3,3,5-trimethyl-	142 C10H22	007154-80-5	78
2	Octane, 3,3-dimethyl-	142 C10H22	004110-44-5	78
3	Heptane, 2,5,5-trimethyl-	142 C10H22	001189-99-7	78
4	4-Methyl-3-heptanol, trifluoroac...	226 C10H17F3O2	1000365-51-8	64
5	Octane, 2-bromo-	192 C8H17Br	000557-35-7	59



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN032219\
Data File : VN054590.D
Acq On : 23 Mar 2019 6:55
Operator : JC/SP
Sample : K2045-16
Misc : 5.53uL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 47 Sample Multiplier: 1

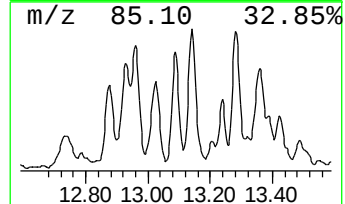
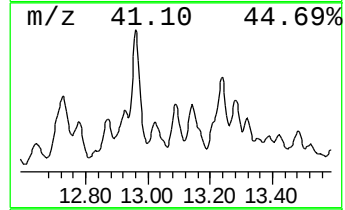
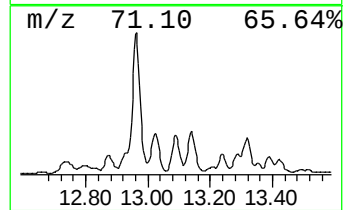
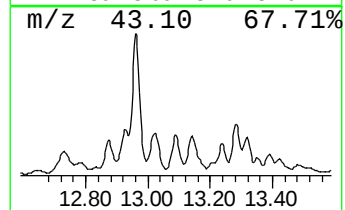
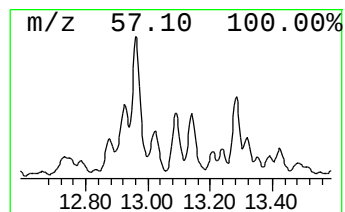
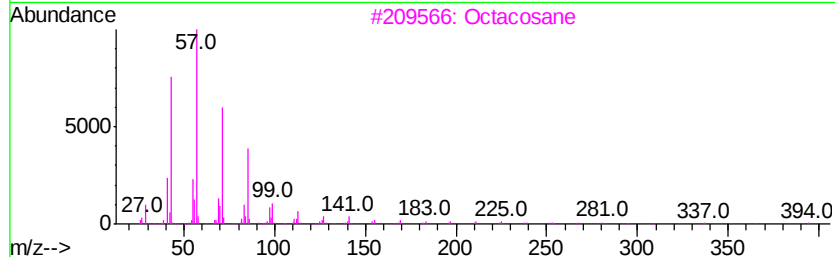
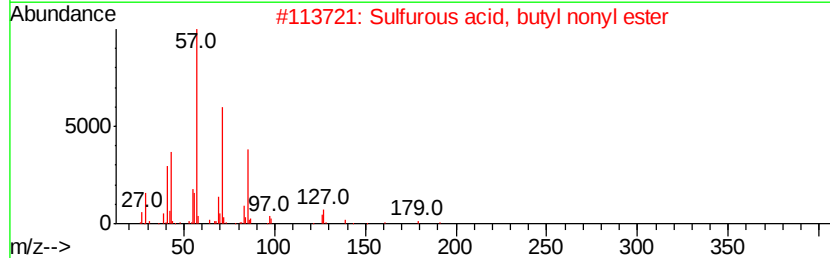
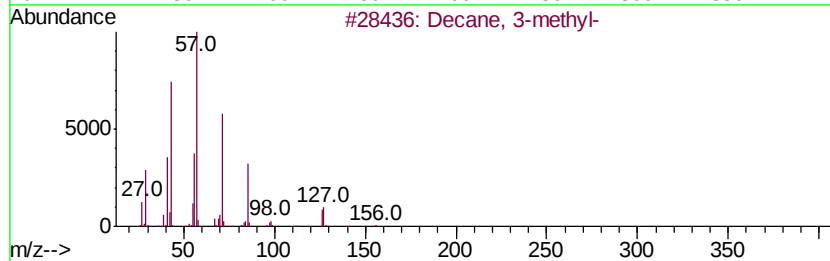
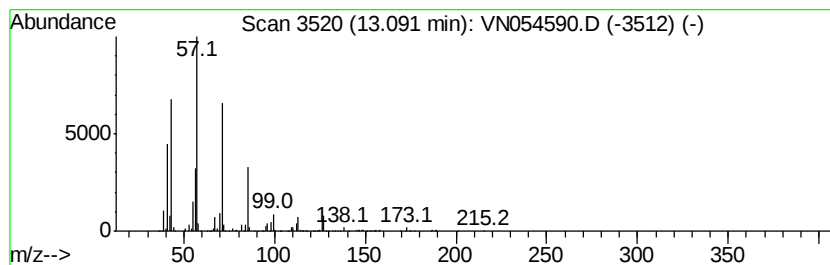
Instrument :
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ClientSampleId :
WP022SB436-190320-(24-26)

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 Decane, 3-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.09	5.93 ug/l	666688	1,4-Dichlorobenzene-d4	13.34
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Decane, 3-methyl-	156 C11H24	013151-34-3	87
2	Sulfurous acid, butyl nonyl ester	264 C13H28O3S	1000309-17-6	80
3	Octacosane	394 C28H58	000630-02-4	72
4	Undecane, 3-methyl-	170 C12H26	001002-43-3	72
5	Decane, 3,8-dimethyl-	170 C12H26	017312-55-9	64



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_N\DATA\VN032219\
Data File : VN054590.D
Acq On : 23 Mar 2019 6:55
Operator : JC/SP
Sample : K2045-16
Misc : 5.53uL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 47 Sample Multiplier: 1

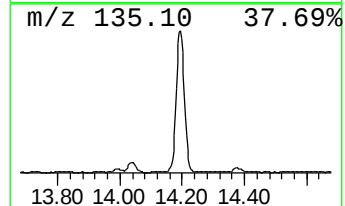
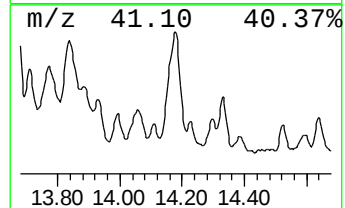
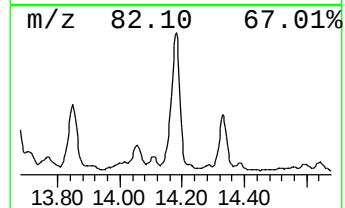
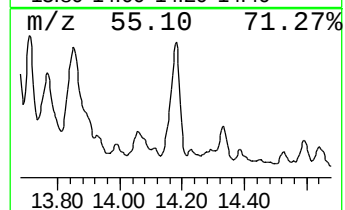
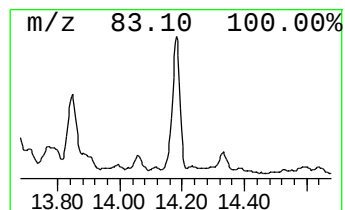
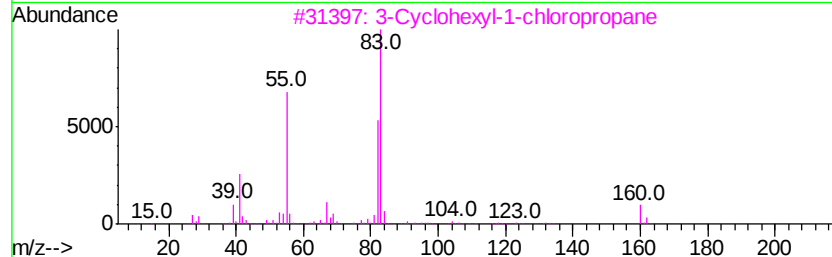
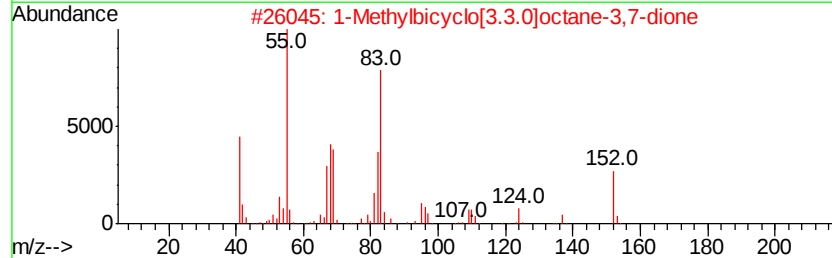
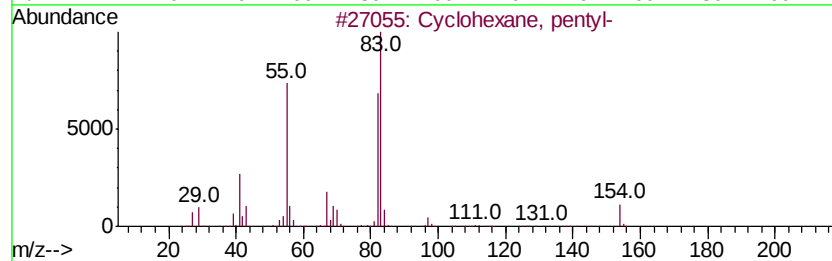
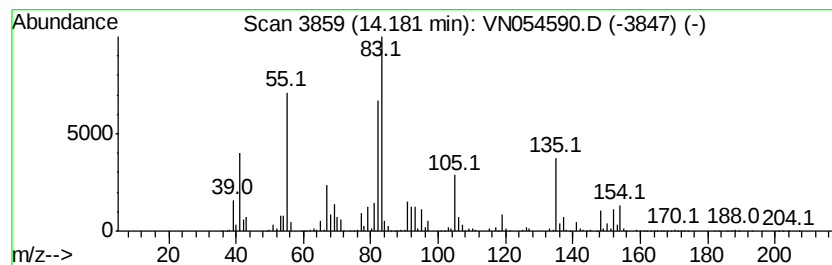
Instrument :
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ClientSampleId :
WP022SB436-190320-(24-26)

Quant Method : Z:\V0ASRV\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 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.18	22.98 ug/l	2584800	1,4-Dichlorobenzene-d4	13.34
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Cyclohexane, pentyl-	154 C11H22	004292-92-6 53
2		1-Methylbicyclo[3.3.0]octane-3,7...	152 C9H12O2	021170-08-1 50
3		3-Cyclohexyl-1-chloropropane	160 C9H17Cl	001124-62-5 43
4		Cyclohexane, 1,1'-(1,4-butanediol...	222 C16H30	006165-44-2 43
5		Cyclohexane, (1-methylethyl)-	126 C9H18	000696-29-7 43



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN032219\
Data File : VN054590.D
Acq On : 23 Mar 2019 6:55
Operator : JC/SP
Sample : K2045-16
Misc : 5.53g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 47 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WP022SB436-190320-(24-26)

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
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Nonane, 3-methyl-	12.04	19.1	ug/l	1085320	3	11.41	2833700	50.0
unknown12.16	12.16	16.6	ug/l	943352	3	11.41	2833700	50.0
unknown12.56	12.56	10.2	ug/l	1149150	4	13.34	5624110	50.0
Cyclohexane, 1-et...	12.73	14.0	ug/l	1576250	4	13.34	5624110	50.0
Heptane, 3,3,5-tr...	12.96	18.0	ug/l	2021620	4	13.34	5624110	50.0
Decane, 3-methyl-	13.09	5.9	ug/l	666688	4	13.34	5624110	50.0
Cyclohexane, pentyl-	14.18	23.0	ug/l	2584800	4	13.34	5624110	50.0