

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN121918\
 Data File : VN053030.D
 Acq On : 20 Dec 2018 00:36
 Operator : MD\SY
 Sample : J6411-03 10X
 Misc : 6.03g/5.0mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 37 Sample Multiplier: 28

Instrument :
 MSVOA_N
 ClientSampleId :
 EP1-MW-I(12-13FT)1218

Integration Parameters: RTEINT.P

Integrator: RTE
 Smoothing : ON Filtering: 5
 Sampling : 1 Min Area: 3 % of largest Peak
 Start Thrs: 0.2 Max Peaks: 100
 Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N121818W.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	1788	1809	1820	rBV	688845	1722125	2.03%	0.208%
2	7.667	1820	1833	1853	rVB	1566108	3675613	4.34%	0.445%
3	8.027	1926	1945	1966	rBV	799287	1841286	2.17%	0.223%
4	8.587	2102	2119	2147	rVB	2225655	4612939	5.45%	0.558%
5	10.091	2572	2587	2612	rVB	4114688	7721270	9.12%	0.935%
6	10.432	2685	2693	2709	rVB	754123	1418359	1.68%	0.172%
7	10.532	2710	2724	2732	rBV2	453941	980055	1.16%	0.119%
8	10.628	2745	2754	2763	rVB	669514	1068375	1.26%	0.129%
9	10.718	2763	2782	2794	rVB	3111571	5219340	6.16%	0.632%
10	10.821	2794	2814	2827	rBV	1699351	3790804	4.48%	0.459%
11	10.889	2827	2835	2842	rBV4	776754	1331316	1.57%	0.161%
12	11.008	2860	2872	2882	rBV	6967950	12993793	15.35%	1.573%
13	11.059	2883	2888	2895	rVB	844921	1125135	1.33%	0.136%
14	11.123	2896	2908	2916	rBV5	3930269	7258625	8.57%	0.879%
15	11.197	2916	2931	2951	rVB5	5309912	16618701	19.63%	2.011%
16	11.300	2951	2963	2985	rBV	7659861	14115786	16.67%	1.708%
17	11.406	2986	2996	3005	rBV	3033274	5350211	6.32%	0.648%
18	11.506	3016	3027	3031	rBV3	1007422	1966651	2.32%	0.238%
19	11.545	3032	3039	3045	rVV	2604709	4160613	4.91%	0.504%
20	11.593	3045	3054	3063	rVV6	4553917	10013559	11.83%	1.212%
21	11.654	3064	3073	3081	rVV2	10165148	19426876	22.94%	2.351%
22	11.699	3082	3087	3097	rVB3	6981818	10891323	12.86%	1.318%
23	11.760	3097	3106	3113	rBV3	1661185	3114333	3.68%	0.377%
24	11.853	3128	3135	3143	rVB4	2560034	3794677	4.48%	0.459%
25	11.924	3143	3157	3169	rBV6	11986206	29785205	35.18%	3.605%
26	12.046	3187	3195	3203	rBV	14626838	20440331	24.14%	2.474%
27	12.120	3210	3218	3223	rBV3	10248449	16098937	19.01%	1.949%
28	12.165	3224	3232	3249	rVV4	20206992	41057300	48.49%	4.969%
29	12.249	3252	3258	3264	rVV3	4995149	7472228	8.82%	0.904%
30	12.297	3267	3273	3280	rVV5	6821801	12990928	15.34%	1.572%
31	12.336	3281	3285	3296	rVB2	13279157	19607664	23.16%	2.373%
32	12.403	3297	3306	3315	rBV6	4602158	8615257	10.17%	1.043%
33	12.487	3316	3332	3339	rBV8	3427025	10531227	12.44%	1.275%
34	12.564	3348	3356	3363	rBV2	14145951	24840994	29.34%	3.007%

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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 >
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35	12.647	3372	3382	3389	rBV5	7033677	14279869	16.86%	1.728%
36	12.731	3389	3408	3417	rVV6	28022412	78887865	93.16%	9.548%
37	12.783	3418	3424	3434	rVB3	11220307	17603850	20.79%	2.131%
38	12.869	3444	3451	3458	rBV3	5163596	7032555	8.31%	0.851%
39	12.908	3459	3463	3466	rBV2	2253955	2356912	2.78%	0.285%
40	12.963	3473	3480	3494	rVB3	15874795	27668401	32.68%	3.349%
41	13.043	3494	3505	3515	rBV2	50897211	84676670	100.00%	10.249%
42	13.172	3533	3545	3552	rVB6	8221672	15976360	18.87%	1.934%
43	13.239	3553	3566	3574	rBV3	18618721	35898461	42.39%	4.345%
44	13.374	3602	3608	3624	rVB	8139753	12875644	15.21%	1.558%
45	13.516	3647	3652	3654	rBV	2904132	2977122	3.52%	0.360%
46	13.590	3667	3675	3689	rVB4	14251186	29997184	35.43%	3.631%
47	13.664	3690	3698	3708	rVB4	12799205	21900348	25.86%	2.651%
48	13.802	3735	3741	3746	rBV2	6705730	9918641	11.71%	1.200%
49	13.834	3747	3751	3760	rVV	9636481	13408079	15.83%	1.623%
50	13.889	3761	3768	3778	rVB	13918930	21715718	25.65%	2.628%
51	13.995	3792	3801	3811	rVB3	12163599	20562882	24.28%	2.489%
52	14.072	3811	3825	3833	rBV6	2786078	7451636	8.80%	0.902%
53	14.175	3849	3857	3863	rBV4	4319551	7668876	9.06%	0.928%
54	14.249	3874	3880	3888	rVB	7798277	11075537	13.08%	1.341%
55	14.294	3888	3894	3900	rBV3	3244596	4120509	4.87%	0.499%
56	14.332	3900	3906	3914	rVB2	3573037	4611909	5.45%	0.558%
57	14.432	3933	3937	3945	rVB2	2503313	3283686	3.88%	0.397%
58	14.480	3945	3952	3960	rVV4	1521174	3340397	3.94%	0.404%
59	14.525	3961	3966	3974	rVB2	2755654	3799024	4.49%	0.460%
60	14.583	3974	3984	3997	rVB2	8620900	16077505	18.99%	1.946%
61	14.651	3997	4005	4014	rBV	1476504	2379815	2.81%	0.288%
62	14.741	4025	4033	4042	rVB	3166894	4582275	5.41%	0.555%
63	14.853	4061	4068	4073	rBV3	1037352	1497240	1.77%	0.181%
64	14.956	4091	4100	4118	rVB2	1313987	2934298	3.47%	0.355%

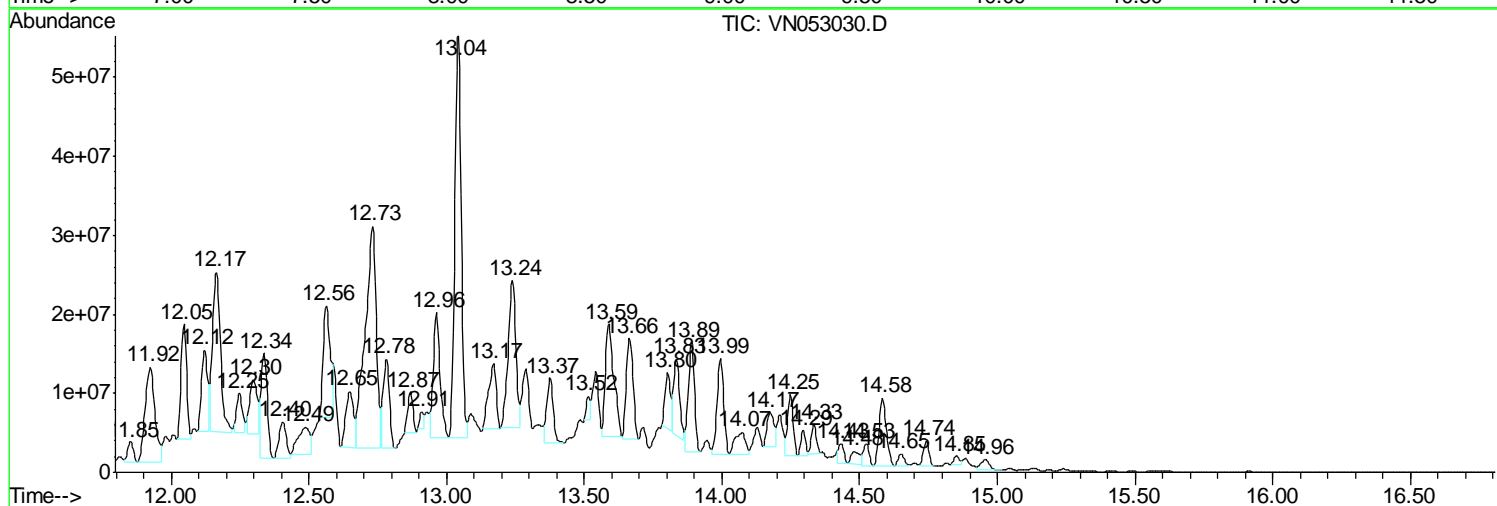
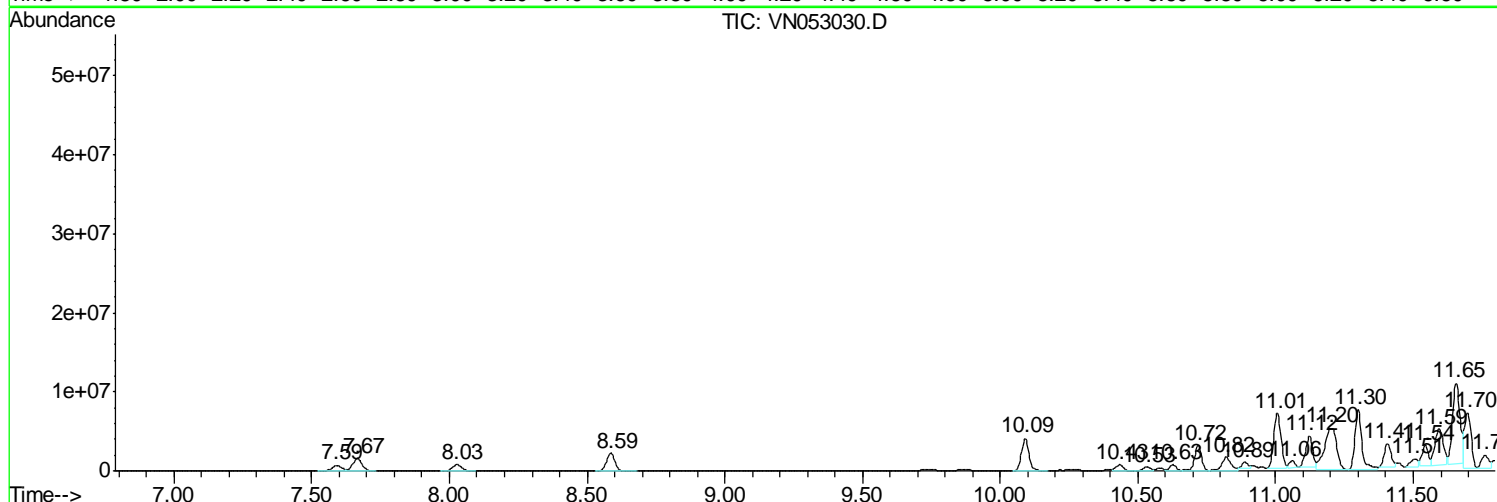
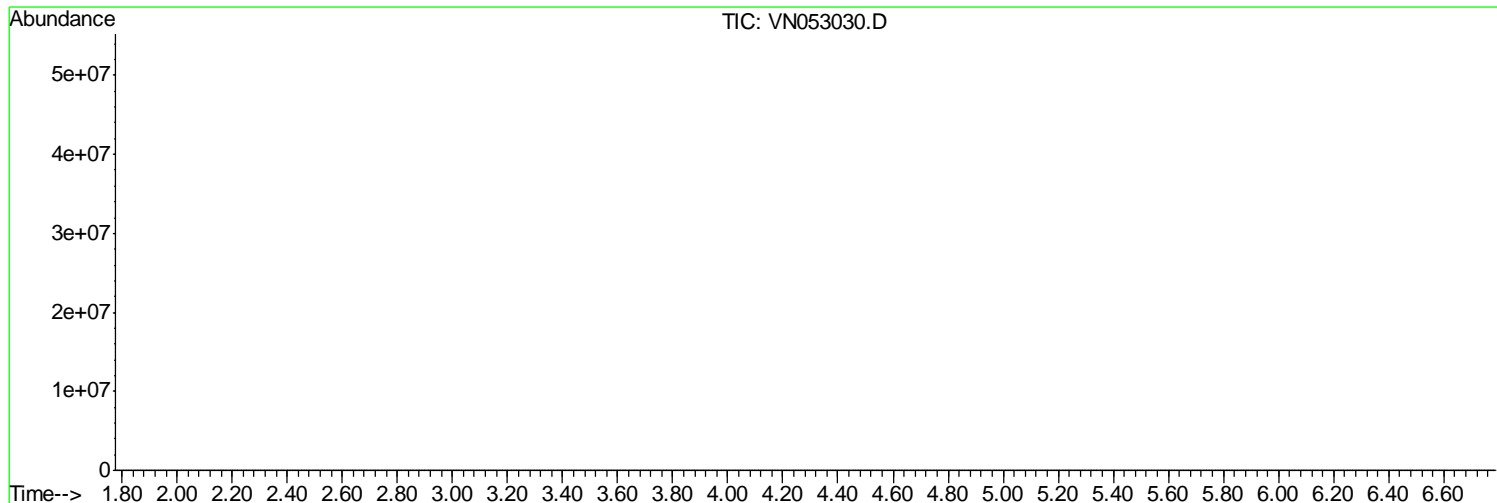
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N121818W.M
 Quant Title : SW846 8260

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



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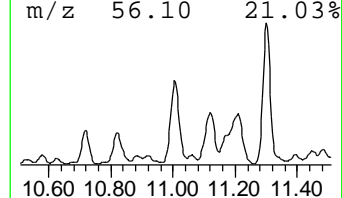
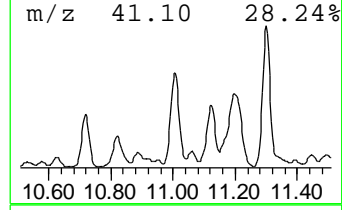
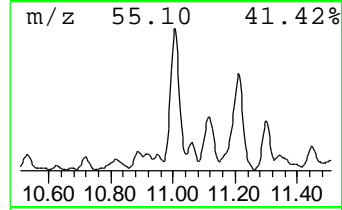
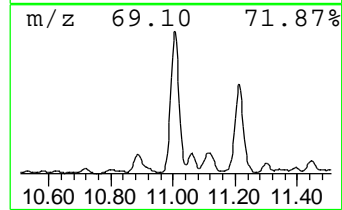
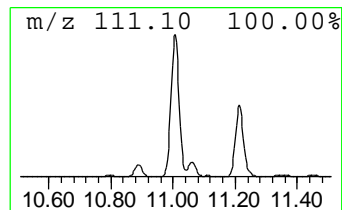
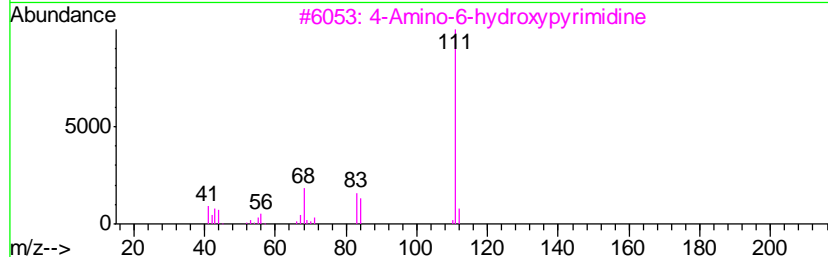
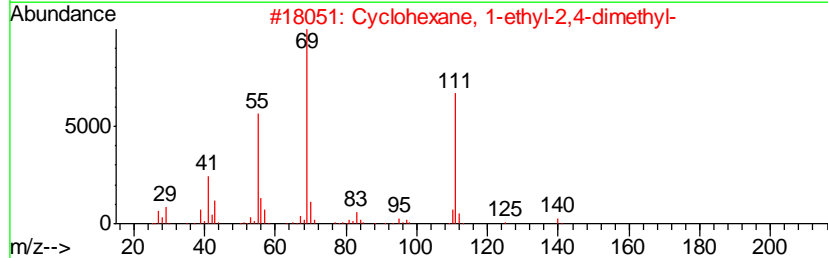
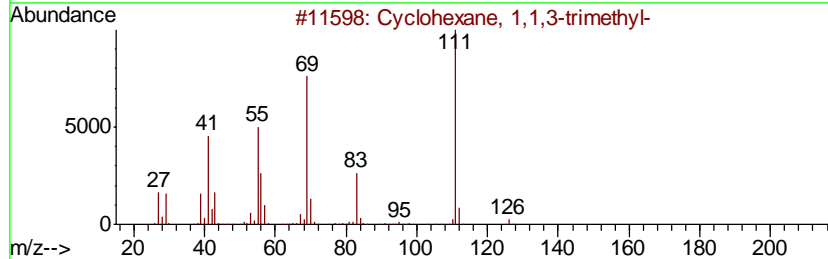
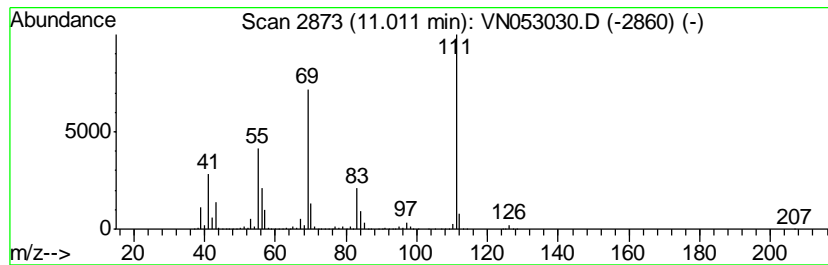
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N121818W.M
 Quant Title : SW846 8260

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

 Peak Number 1 Cyclohexane, 1,1,3-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.01	121.43 ug/l	12993800	Chlorobenzene-d5	11.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, 1,1,3-trimethyl-	126	C9H18	003073-66-3	95
2		Cyclohexane, 1-ethyl-2,4-dimethyl-	140	C10H20	061142-69-6	72
3		4-Amino-6-hydroxypyrimidine	111	C4H5N3O	001193-22-2	50
4		p-Fluoroaniline	111	C6H6FN	000371-40-4	50
5		Benzenamine, 2-fluoro-	111	C6H6FN	000348-54-9	50



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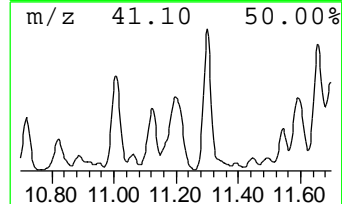
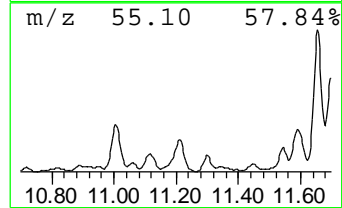
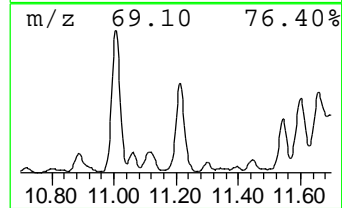
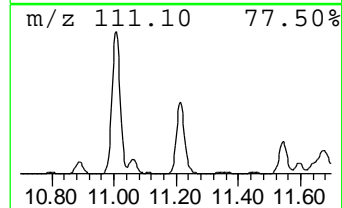
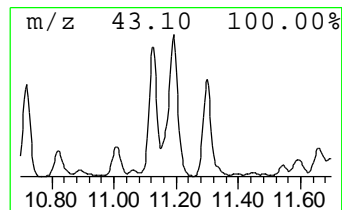
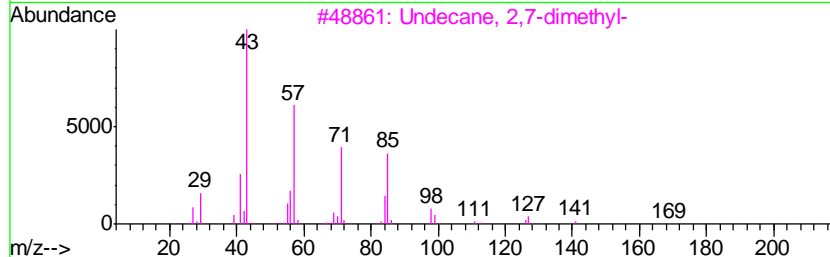
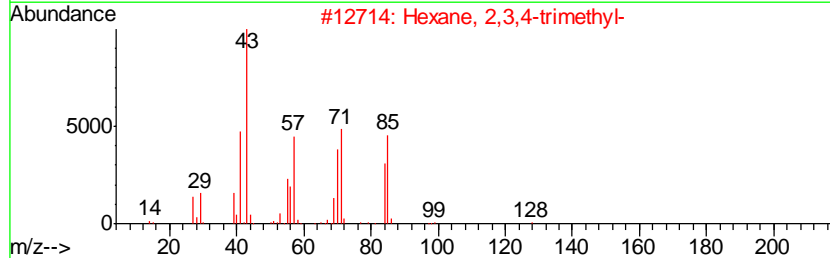
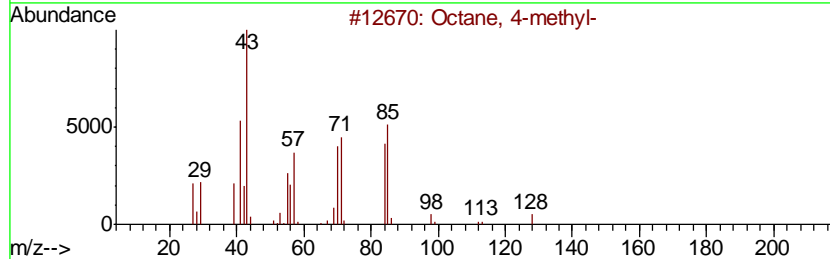
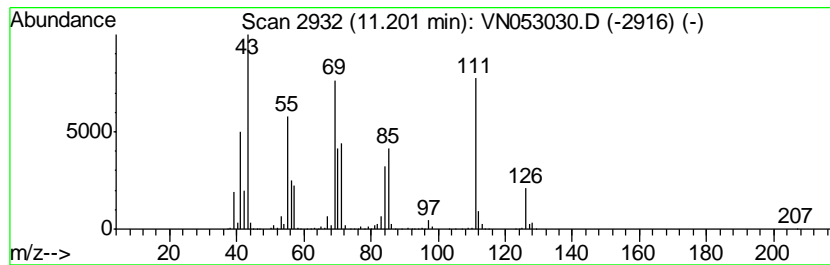
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TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 2 Octane, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.20	155.31 ug/l	16618700	Chlorobenzene-d5	11.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octane, 4-methyl-	128	C9H20	002216-34-4	64
2		Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	53
3		Undecane, 2,7-dimethyl-	184	C13H28	017301-24-5	47
4		Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	43
5		Hexane, 3-ethyl-	114	C8H18	000619-99-8	43



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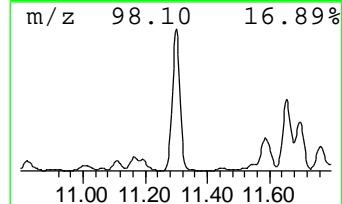
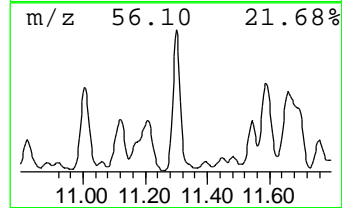
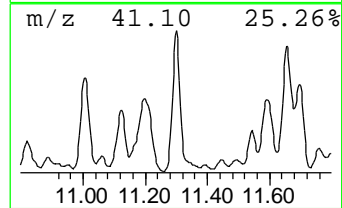
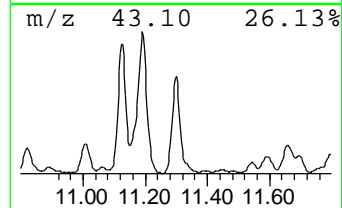
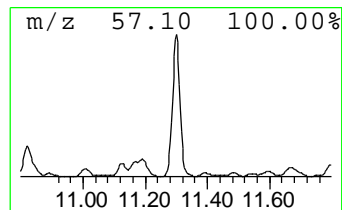
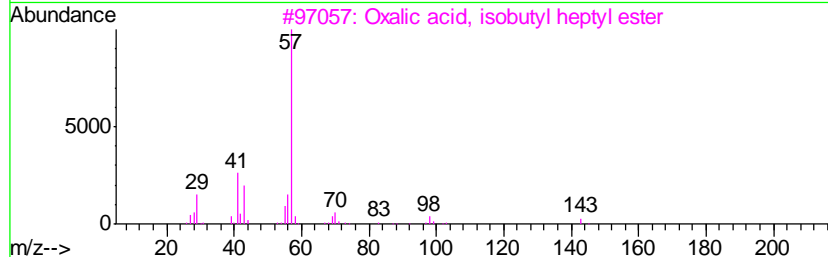
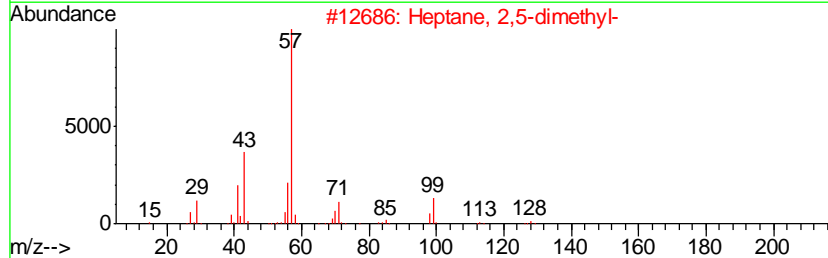
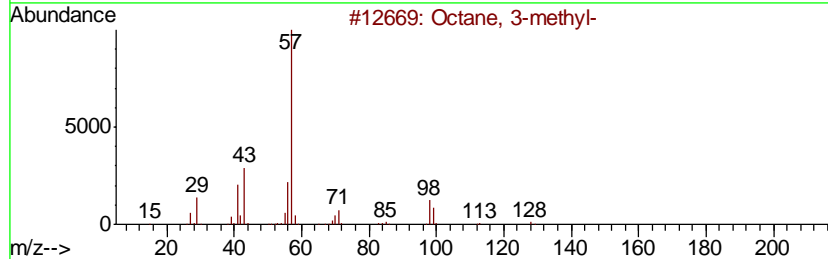
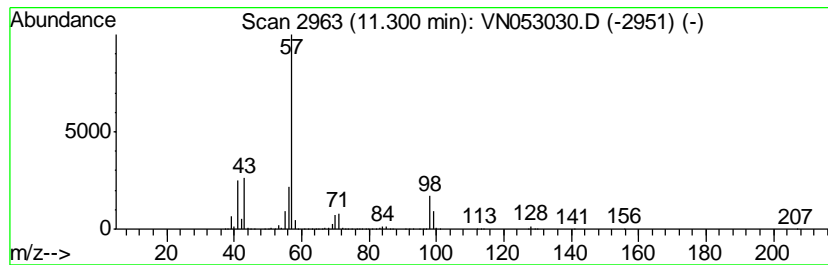
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TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 3 Octane, 3-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.30	131.92 ug/l	14115800	Chlorobenzene-d5	11.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octane, 3-methyl-	128	C9H20	002216-33-3	91
2		Heptane, 2,5-dimethyl-	128	C9H20	002216-30-0	90
3		Oxalic acid, isobutyl heptyl ester	244	C13H24O4	1000309-37-2	53
4		Undecane, 6-methyl-	170	C12H26	017302-33-9	53
5		Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	50



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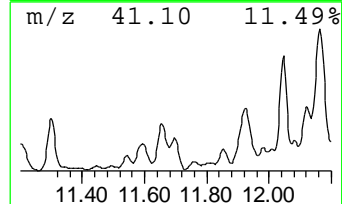
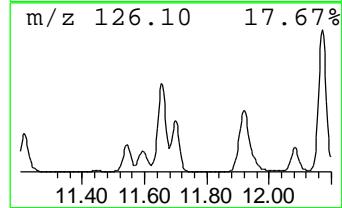
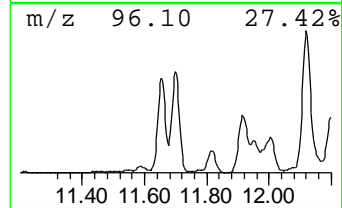
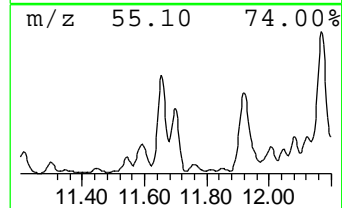
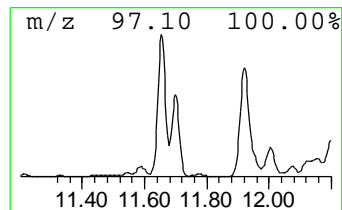
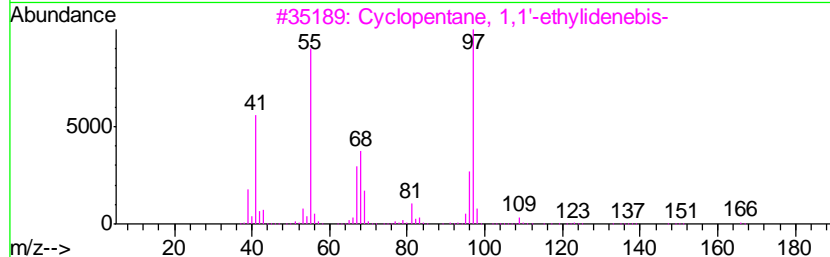
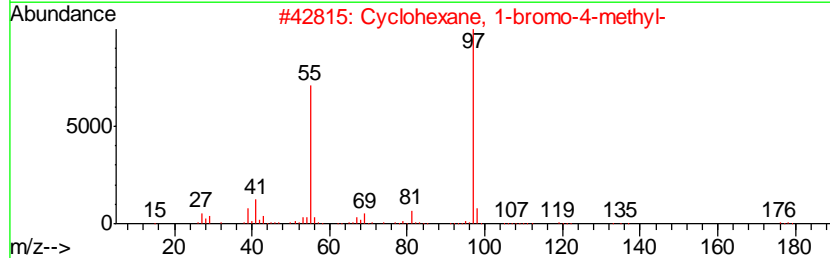
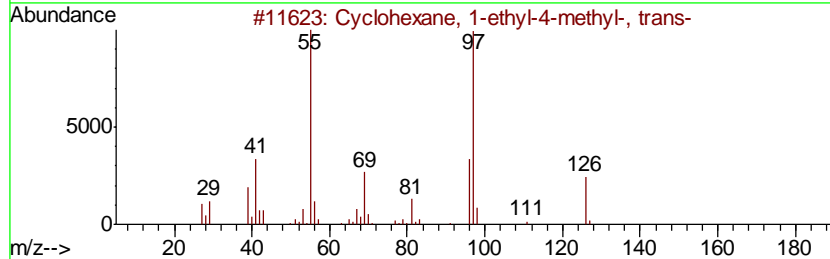
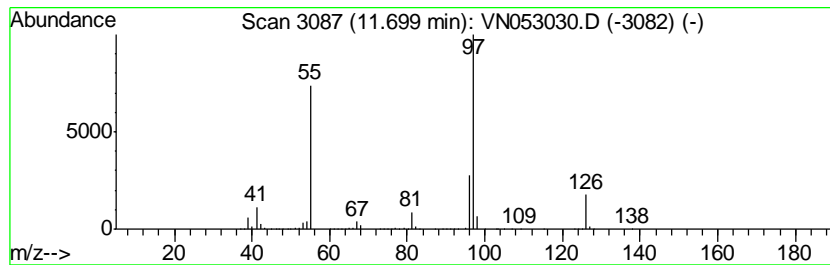
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 Quant Title : SW846 8260

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

 Peak Number 4 Cyclohexane, 1-ethyl-4-meth... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.70	101.78 ug/l	10891300	Chlorobenzene-d5	11.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	006236-88-0	86
2		Cyclohexane, 1-bromo-4-methyl-	176	C7H13Br	006294-40-2	59
3		Cyclopentane, 1,1'-ethylidenebis-	166	C12H22	004413-21-2	56
4		cis-1-Ethyl-3-methyl-cyclohexane	126	C9H18	019489-10-2	56
5		4-Octen-3-one	126	C8H14O	014129-48-7	53



Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN121918\
 Data File : VN053030.D
 Acq On : 20 Dec 2018 00:36
 Operator : MD\SY
 Sample : J6411-03 10X
 Misc : 6.03µ/5.0mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 37 Sample Multiplier: 28

Instrument :
 MSVOA_N
 ClientSampled :
 EP1-MW-I(12-13FT)1218

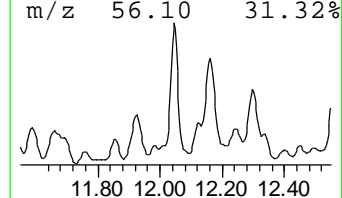
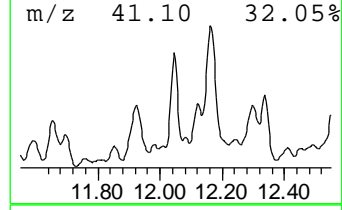
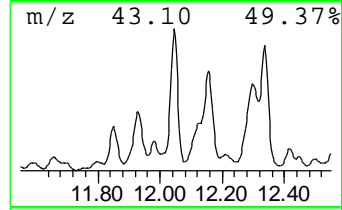
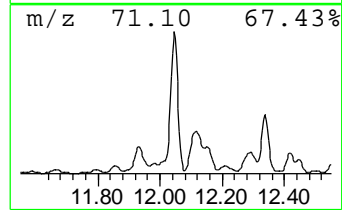
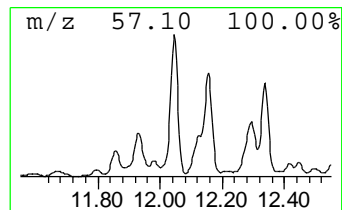
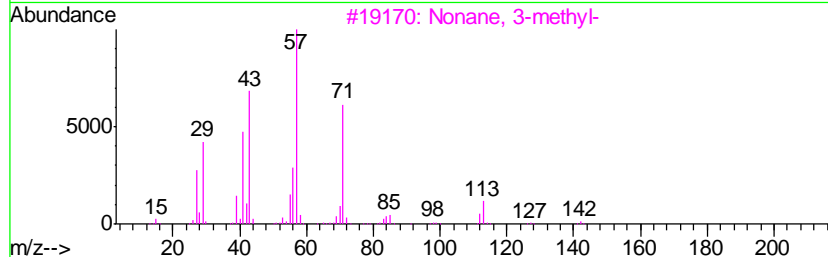
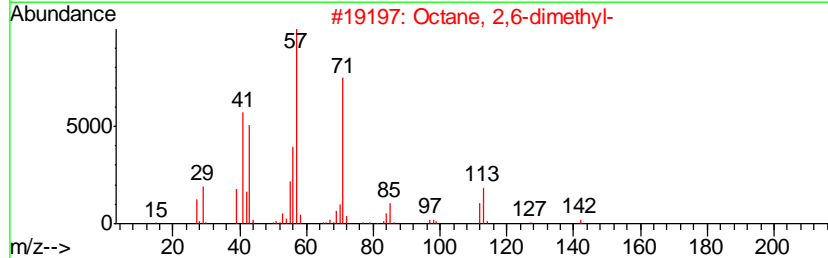
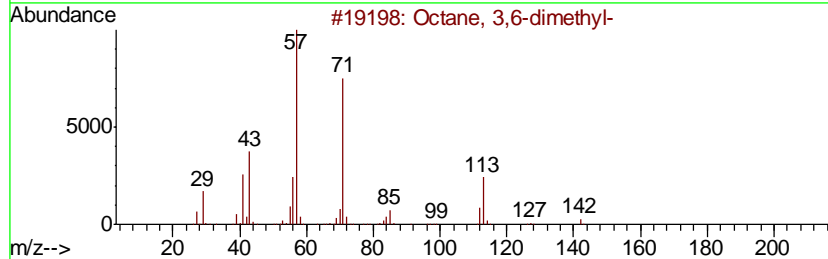
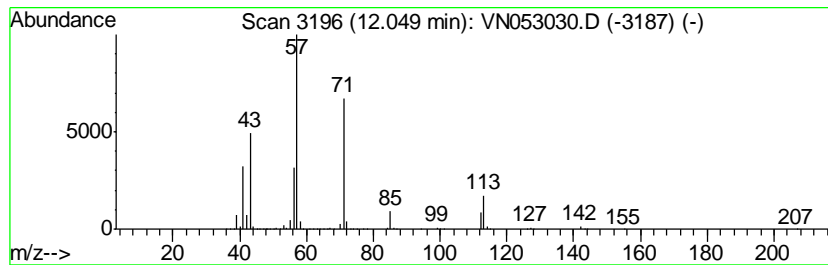
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 Quant Title : SW846 8260

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

 Peak Number 5 Octane, 3,6-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.05	191.02 ug/l	20440300	Chlorobenzene-d5	11.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	91
2		Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	91
3		Nonane, 3-methyl-	142	C10H22	005911-04-6	91
4		Sulfurous acid, 2-ethylhexyl non...	320	C17H36O3S	1000309-19-2	64
5		Undecane, 6,6-dimethyl-	184	C13H28	017312-76-4	64



Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN121918\
 Data File : VN053030.D
 Acq On : 20 Dec 2018 00:36
 Operator : MD\SY
 Sample : J6411-03 10X
 Misc : 6.03µ/5.0mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 37 Sample Multiplier: 28

Instrument :
 MSVOA_N
 ClientSampleId :
 EP1-MW-I(12-13FT)1218

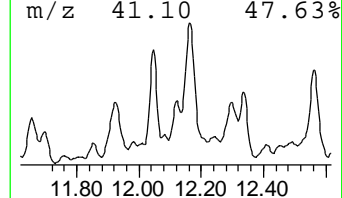
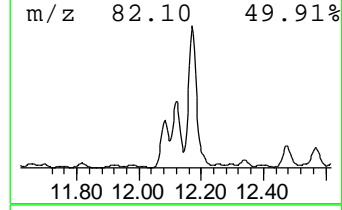
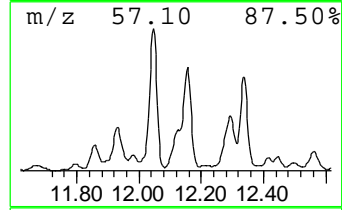
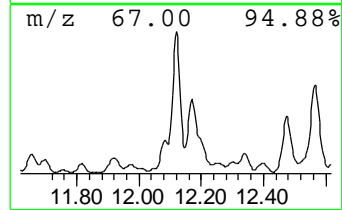
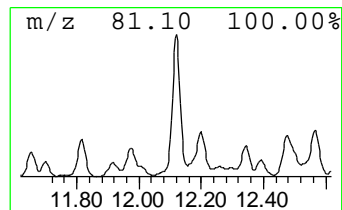
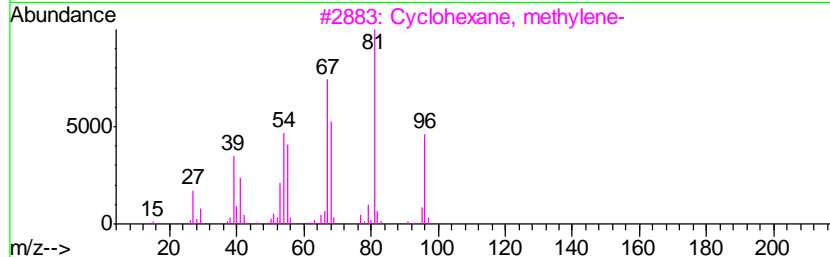
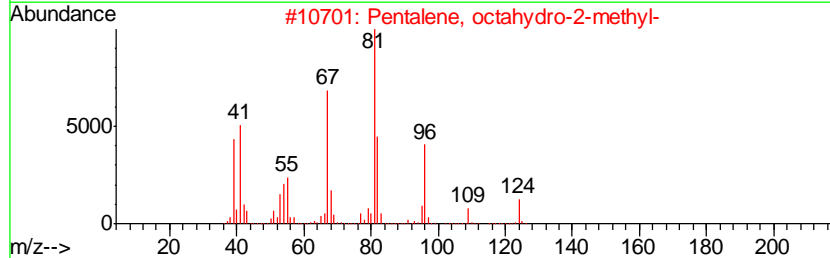
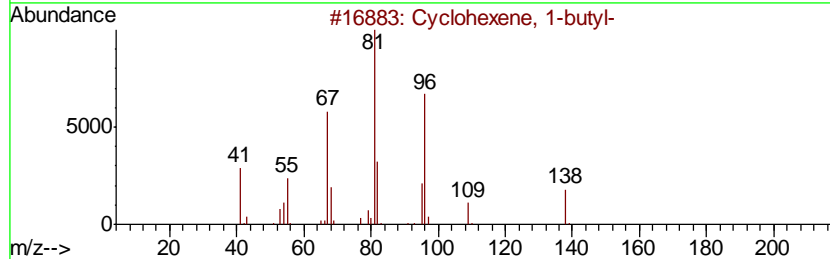
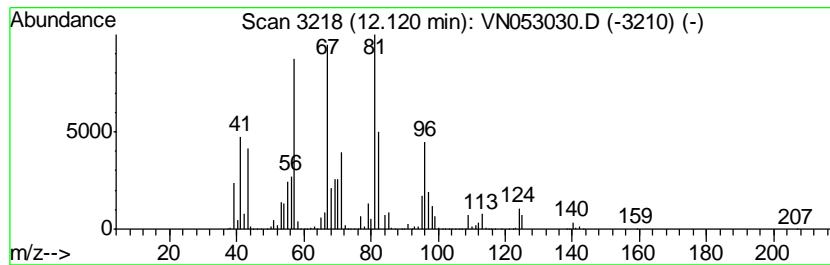
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 Quant Title : SW846 8260

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

 Peak Number 6 Cyclohexene, 1-butyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.12	150.45 ug/l	16098900	Chlorobenzene-d5	11.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexene, 1-butyl-	138	C10H18	003282-53-9	58
2		Pentalene, octahydro-2-methyl-	124	C9H16	003868-64-2	53
3		Cyclohexane, methylene-	96	C7H12	001192-37-6	49
4		1H-Indene, octahydro-, trans-	124	C9H16	003296-50-2	49
5		Bicyclo[3.3.1]nonane	124	C9H16	000280-65-9	46



Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN121918\
 Data File : VN053030.D
 Acq On : 20 Dec 2018 00:36
 Operator : MD\SY
 Sample : J6411-03 10X
 Misc : 6.03µ/5.0mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 37 Sample Multiplier: 28

Instrument :
 MSVOA_N
 ClientSampleID :
 EP1-MW-I(12-13FT)1218

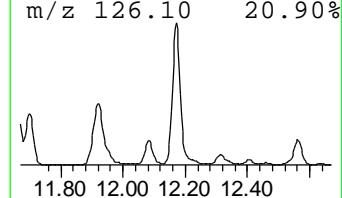
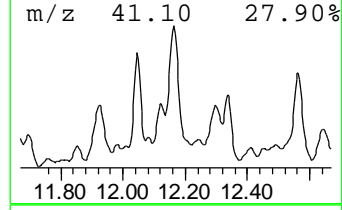
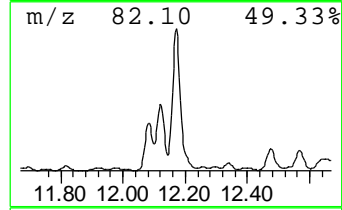
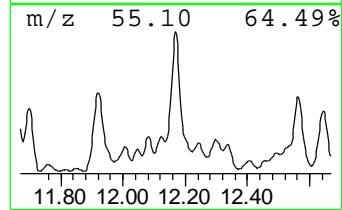
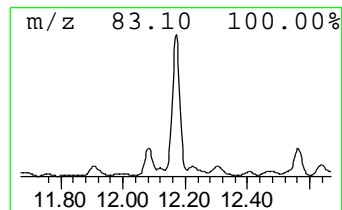
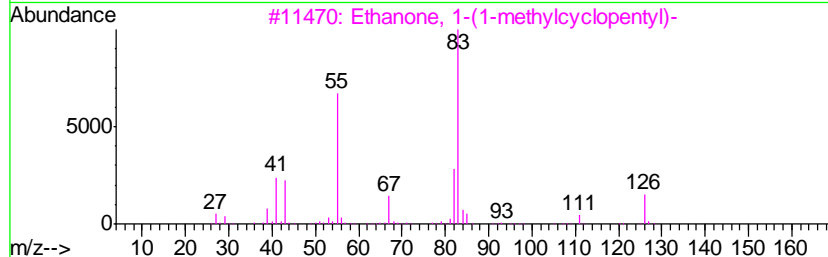
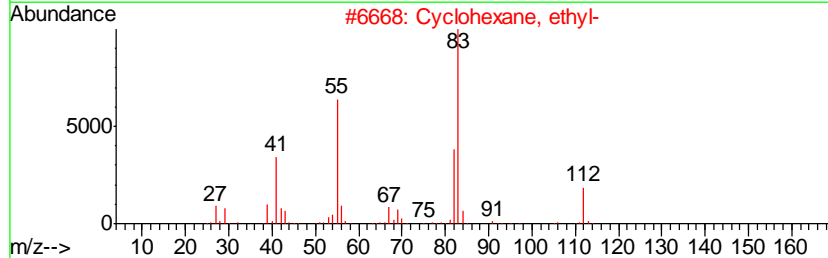
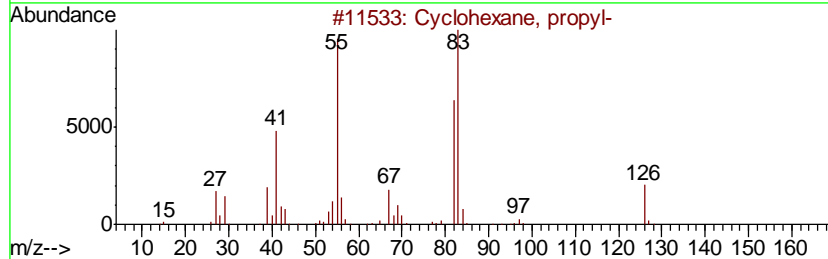
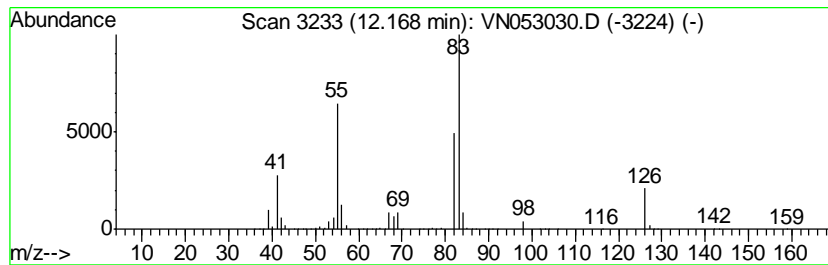
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 Quant Title : SW846 8260

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

 Peak Number 7 Cyclohexane, propyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.17	383.70 ug/l	41057300	Chlorobenzene-d5	11.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, propyl-	126	C9H18	001678-92-8	86
2		Cyclohexane, ethyl-	112	C8H16	001678-91-7	64
3		Ethanone, 1-(1-methylcyclopentyl)-	126	C8H14O	013388-93-7	53
4		Cyclopentane, 1-ethyl-1-methyl-	112	C8H16	016747-50-5	53
5		1-Butene, 2,3,3-trimethyl-	98	C7H14	000594-56-9	52



Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN121918\
 Data File : VN053030.D
 Acq On : 20 Dec 2018 00:36
 Operator : MD\SY
 Sample : J6411-03 10X
 Misc : 6.03µ/5.0mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 37 Sample Multiplier: 28

Instrument :
 MSVOA_N
 ClientSampled :
 EP1-MW-I(12-13FT)1218

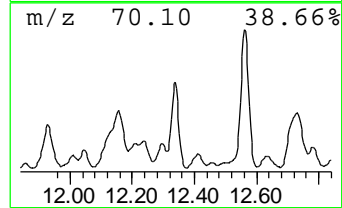
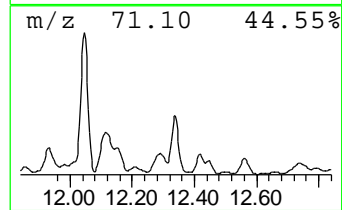
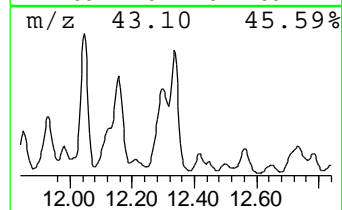
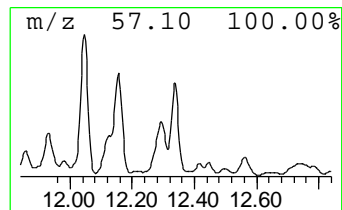
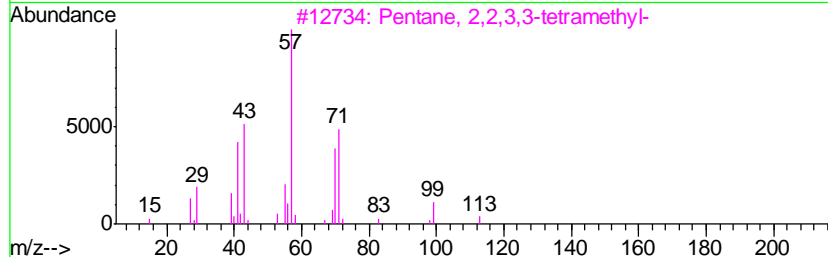
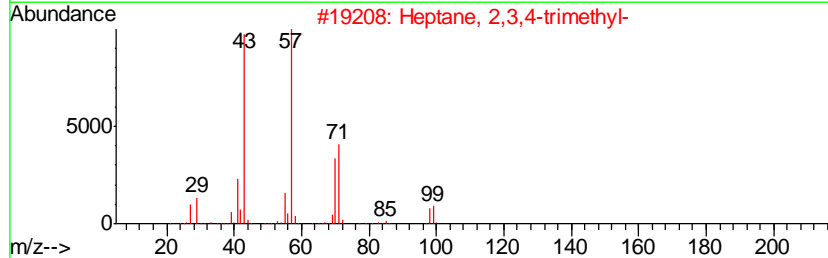
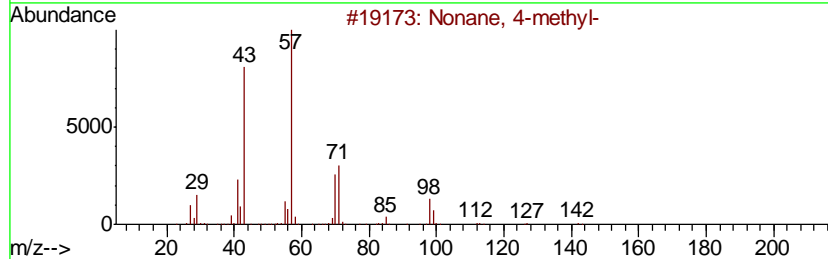
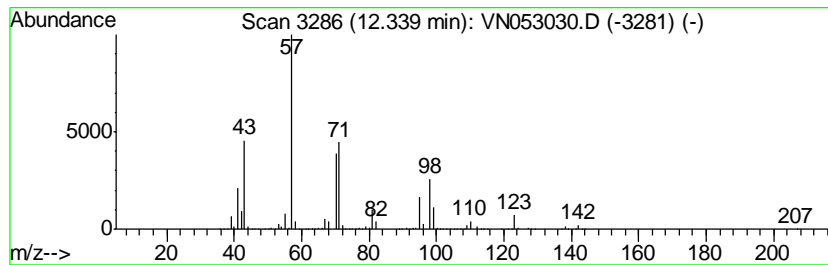
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 Quant Title : SW846 8260

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

 Peak Number 8 Nonane, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.34	183.24 ug/l	19607700	Chlorobenzene-d5	11.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonane, 4-methyl-	142	C10H22	017301-94-9	72
2		Heptane, 2,3,4-trimethyl-	142	C10H22	052896-95-4	53
3		Pentane, 2,2,3,3-tetramethyl-	128	C9H20	007154-79-2	53
4		Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	49
5		Undecane, 4,5-dimethyl-	184	C13H28	017312-79-7	40



Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN121918\
 Data File : VN053030.D
 Acq On : 20 Dec 2018 00:36
 Operator : MD\SY
 Sample : J6411-03 10X
 Misc : 6.03µ/5.0mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 37 Sample Multiplier: 28

Instrument :
 MSVOA_N
 ClientSampleId :
 EP1-MW-I(12-13FT)1218

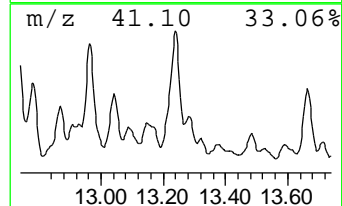
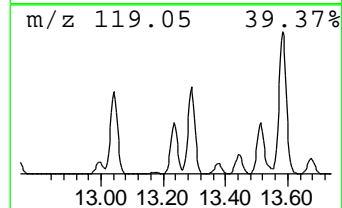
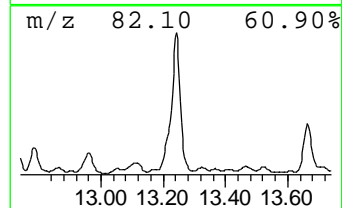
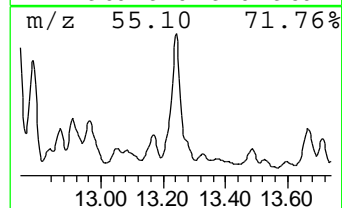
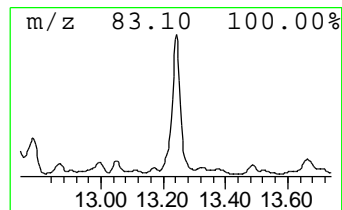
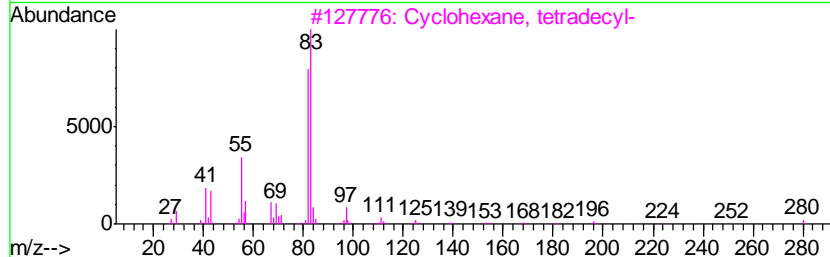
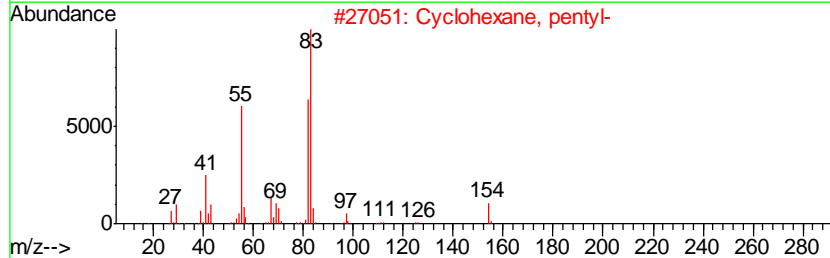
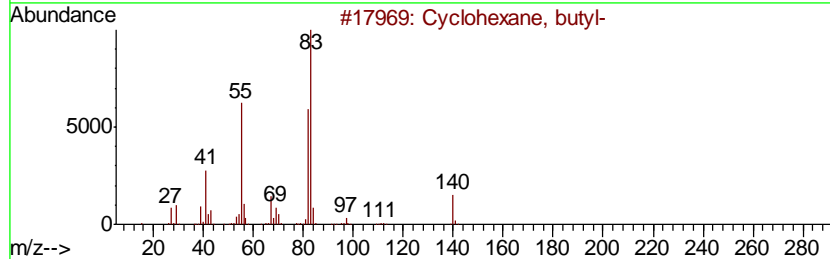
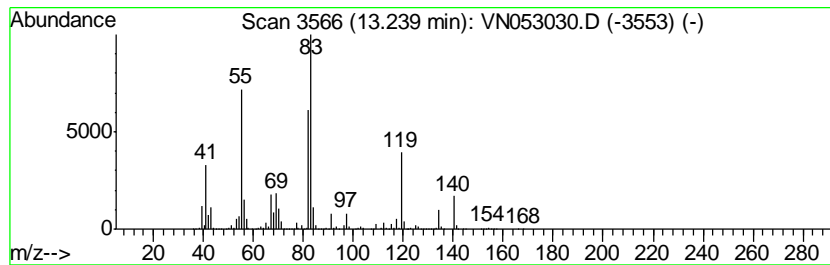
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 Quant Title : SW846 8260

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

 Peak Number 9 Cyclohexane, butyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.24	139.41 ug/l	35898500	1,4-Dichlorobenzene-d4	13.34

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, butyl-	140	C10H20	001678-93-9	92
2		Cyclohexane, pentyl-	154	C11H22	004292-92-6	64
3		Cyclohexane, tetradecyl-	280	C20H40	001795-18-2	50
4		Cyclohexane, decyl-	224	C16H32	001795-16-0	50
5		Cyclohexane, (2-methylpropyl)-	140	C10H20	001678-98-4	50



Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN121918\
 Data File : VN053030.D
 Acq On : 20 Dec 2018 00:36
 Operator : MD\SY
 Sample : J6411-03 10X
 Misc : 6.03µ/5.0mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 37 Sample Multiplier: 28

Instrument :
 MSVOA_N
 ClientSampleId :
 EP1-MW-I(12-13FT)1218

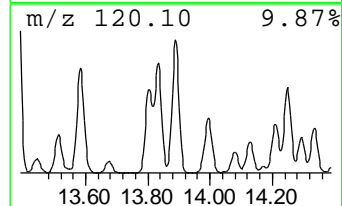
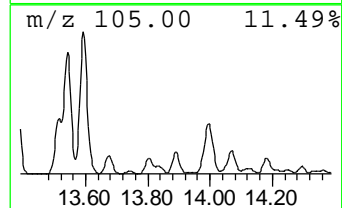
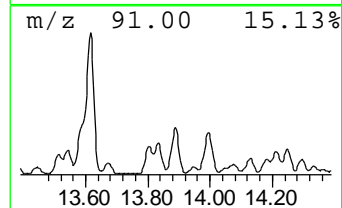
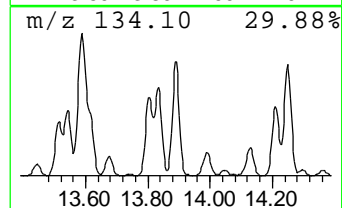
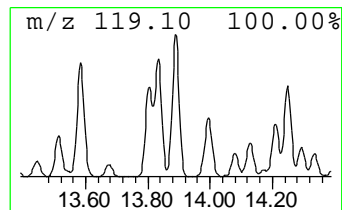
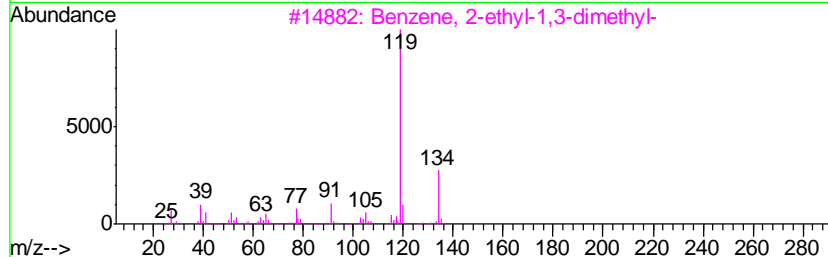
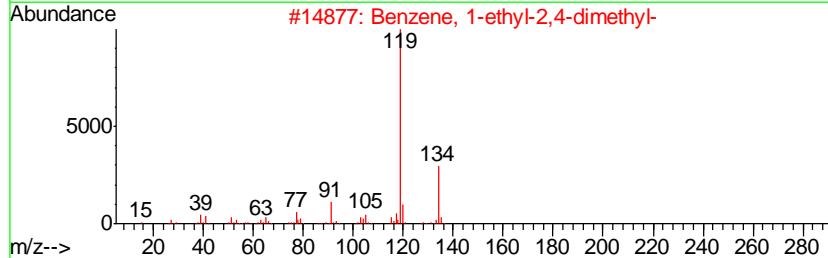
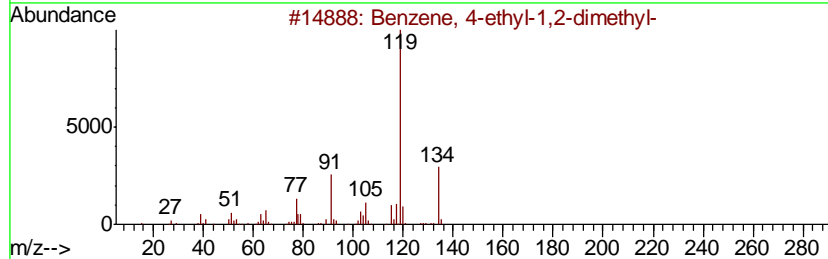
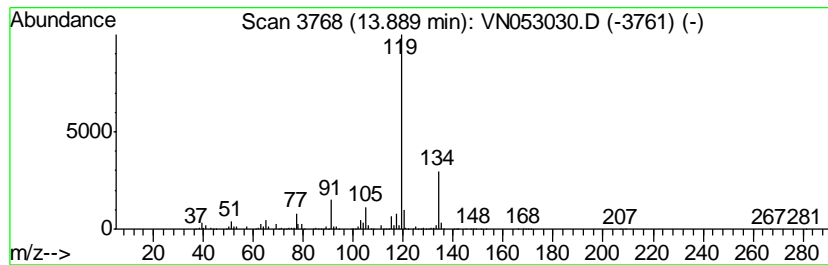
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 Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	84.33 ug/l	21715700	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	96
2		Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	95
3		Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	95
4		Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95
5		o-Cymene	134	C10H14	000527-84-4	95



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN121918\
 Data File : VN053030.D
 Acq On : 20 Dec 2018 00:36
 Operator : MD\SY
 Sample : J6411-03 10X
 Misc : 6.03g/5.0mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 37 Sample Multiplier: 28

Instrument :
 MSVOA_N
 ClientSampleId :
 EP1-MW-I(12-13FT)1218

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N121818W.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,...	11.01	121.4	ug/l	12993800	3	11.41	5350210	50.0
Octane, 4-methyl-	11.20	155.3	ug/l	16618700	3	11.41	5350210	50.0
Octane, 3-methyl-	11.30	131.9	ug/l	14115800	3	11.41	5350210	50.0
Cyclohexane, 1-et...	11.70	101.8	ug/l	10891300	3	11.41	5350210	50.0
Octane, 3,6-dimet...	12.05	191.0	ug/l	20440300	3	11.41	5350210	50.0
Cyclohexene, 1-bu...	12.12	150.4	ug/l	16098900	3	11.41	5350210	50.0
Cyclohexane, propyl-	12.17	383.7	ug/l	41057300	3	11.41	5350210	50.0
Nonane, 4-methyl-	12.34	183.2	ug/l	19607700	3	11.41	5350210	50.0
Cyclohexane, butyl-	13.24	139.4	ug/l	35898500	4	13.34	12875600	50.0
Benzene, 4-ethyl-...	13.89	84.3	ug/l	21715700	4	13.34	12875600	50.0