

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN100818\
 Data File : VN051731.D
 Acq On : 8 Oct 2018 13:20
 Operator : MD\SY
 Sample : J5165-05 10X
 Misc : 6.24g/5mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 14 Sample Multiplier: 28

Instrument :
 MSVOA_N
 ClientSampleId :
 EP1-MW-D-092718(7-10)

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\82N100418W.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	1786	1810	1821	rBV2	518043	1306189	3.51%	0.331%
2	7.667	1821	1833	1853	rVB	817045	1922572	5.17%	0.488%
3	8.030	1926	1946	1969	rBV	494778	1172905	3.15%	0.298%
4	8.587	2103	2119	2145	rBV	1096338	2272155	6.11%	0.577%
5	10.091	2573	2587	2610	rBV	2063671	3769968	10.13%	0.957%
6	10.435	2685	2694	2710	rVB	440601	830094	2.23%	0.211%
7	10.532	2710	2724	2733	rBV3	221995	488583	1.31%	0.124%
8	10.628	2746	2754	2763	rVB	313410	493010	1.33%	0.125%
9	10.718	2771	2782	2796	rVB	1633682	2784734	7.49%	0.707%
10	10.821	2797	2814	2828	rBV	870356	1966726	5.29%	0.499%
11	10.892	2828	2836	2841	rBV2	310457	520949	1.40%	0.132%
12	11.008	2856	2872	2883	rBV	4067018	7827311	21.04%	1.986%
13	11.059	2883	2888	2896	rVV	543059	830403	2.23%	0.211%
14	11.123	2896	2908	2916	rVV4	2015978	3728822	10.02%	0.946%
15	11.169	2917	2922	2923	rVV2	580907	591978	1.59%	0.150%
16	11.210	2927	2935	2951	rVB3	2240016	4734866	12.73%	1.202%
17	11.291	2951	2960	2968	rBV	585693	936999	2.52%	0.238%
18	11.410	2986	2997	3005	rBV	1559564	2844306	7.65%	0.722%
19	11.545	3030	3039	3045	rBV	1371174	2206659	5.93%	0.560%
20	11.596	3045	3055	3064	rVV6	2065649	4460793	11.99%	1.132%
21	11.657	3064	3074	3081	rVV	4593061	8851949	23.80%	2.246%
22	11.699	3082	3087	3097	rVB3	3591815	5612548	15.09%	1.424%
23	11.760	3097	3106	3113	rBV3	920743	1708469	4.59%	0.434%
24	11.853	3128	3135	3143	rVB4	1566339	2288751	6.15%	0.581%
25	11.924	3143	3157	3169	rBV5	7113879	17379079	46.72%	4.411%
26	12.046	3187	3195	3203	rBV	10751892	14646358	39.37%	3.717%
27	12.123	3211	3219	3223	rBV6	3701930	5958211	16.02%	1.512%
28	12.156	3224	3229	3237	rVB	6454003	9246755	24.86%	2.347%
29	12.201	3238	3243	3250	rBV5	1376383	2326144	6.25%	0.590%
30	12.403	3296	3306	3317	rBV5	3623559	6809164	18.31%	1.728%
31	12.493	3317	3334	3339	rBV7	2922648	8093433	21.76%	2.054%
32	12.564	3348	3356	3369	rVB4	12468691	23400861	62.91%	5.939%
33	12.648	3370	3382	3391	rBV6	5201163	12065895	32.44%	3.062%
34	12.728	3394	3407	3416	rVV5	14005667	37197519	100.00%	9.440%

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35	12.779	3418	3423	3434	rVB4	7745577	12683315	34.10%	3.219%
36	12.869	3444	3451	3458	rBV4	3921855	5436484	14.62%	1.380%
37	12.927	3459	3469	3472	rVV2	2443589	5076050	13.65%	1.288%
38	12.963	3473	3480	3495	rVB3	13973994	24490595	65.84%	6.215%
39	13.168	3532	3544	3552	rBV6	5961008	12717470	34.19%	3.227%
40	13.242	3553	3567	3576	rBV2	10040696	20281819	54.52%	5.147%
41	13.596	3668	3677	3688	rBV2	6566735	13297168	35.75%	3.375%
42	13.664	3689	3698	3708	rVV5	10830981	19652249	52.83%	4.987%
43	13.802	3735	3741	3748	rVB2	5146161	6087367	16.36%	1.545%
44	13.889	3761	3768	3778	rVB	12509060	19840001	53.34%	5.035%
45	13.988	3792	3799	3811	rVB5	3085135	6499721	17.47%	1.650%
46	14.072	3817	3825	3833	rBV5	2282724	3915690	10.53%	0.994%
47	14.175	3849	3857	3863	rBV5	4399782	8032751	21.59%	2.039%
48	14.249	3874	3880	3888	rVB	8164758	11553559	31.06%	2.932%
49	14.294	3888	3894	3900	rBV3	1932440	2379039	6.40%	0.604%
50	14.332	3901	3906	3912	rVV2	1718505	1964634	5.28%	0.499%
51	14.480	3945	3952	3959	rBV7	1017478	2028357	5.45%	0.515%
52	14.525	3960	3966	3974	rVV	2926389	4226581	11.36%	1.073%
53	14.583	3975	3984	3997	rVV5	2535331	5352020	14.39%	1.358%
54	14.651	3997	4005	4015	rVB2	1696631	2794355	7.51%	0.709%
55	14.853	4061	4068	4072	rBV4	768443	1068028	2.87%	0.271%
56	14.956	4091	4100	4112	rVB3	1354227	2904946	7.81%	0.737%
57	15.046	4121	4128	4137	rVB3	284756	480908	1.29%	0.122%

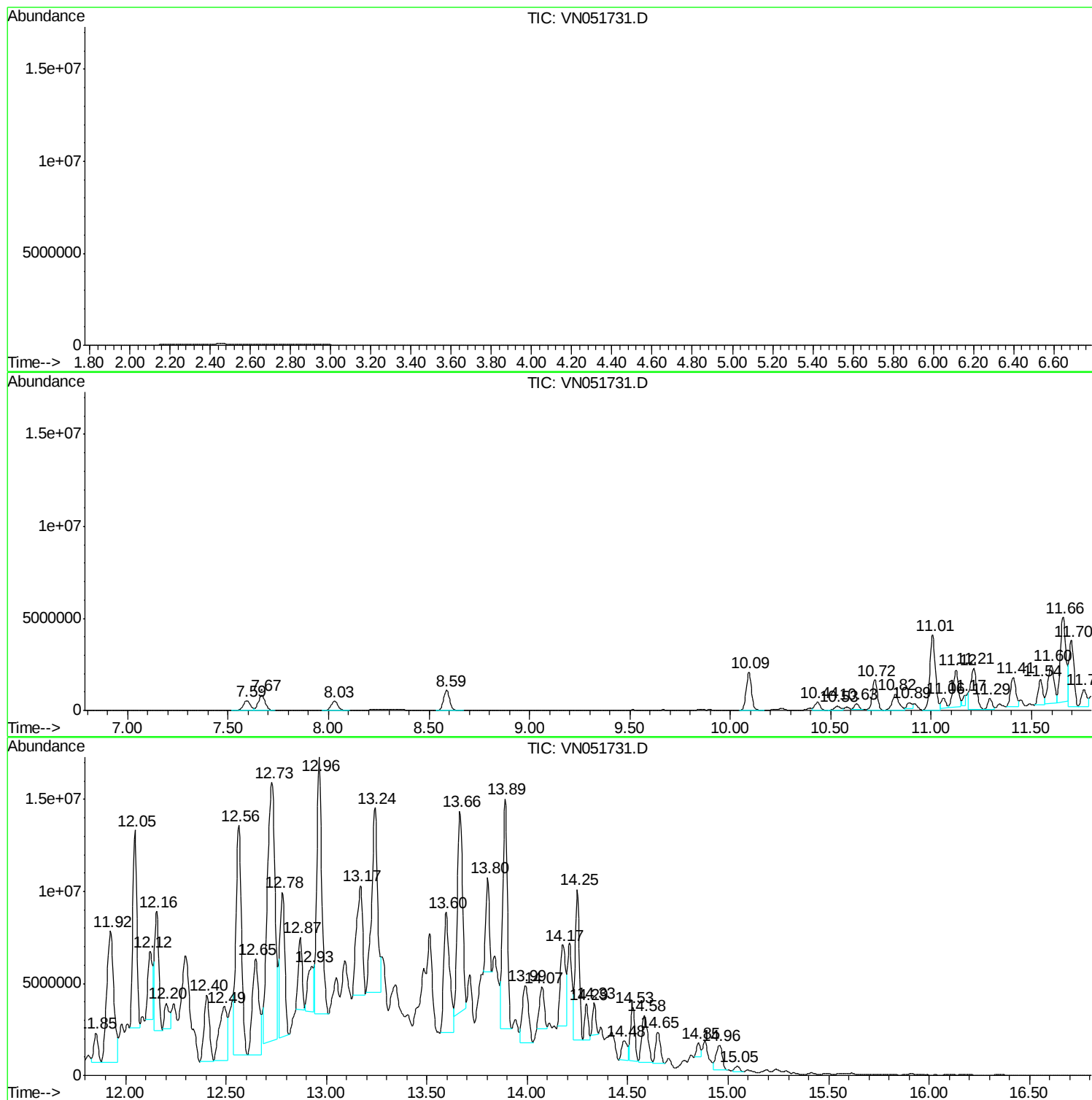
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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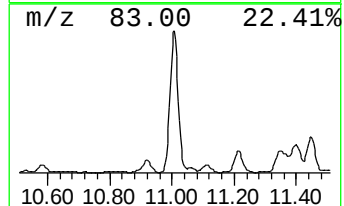
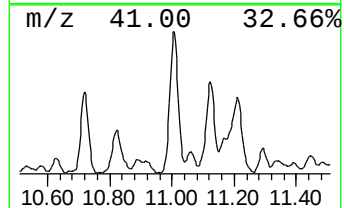
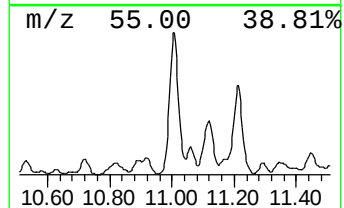
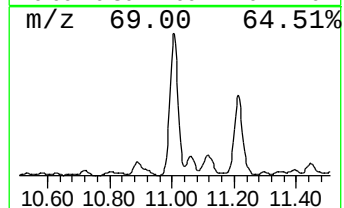
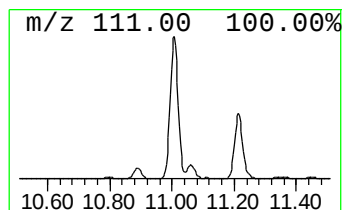
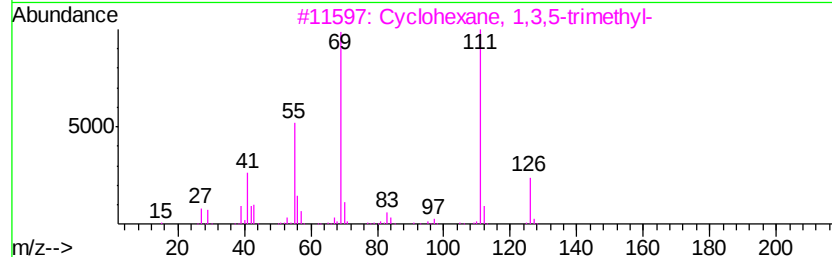
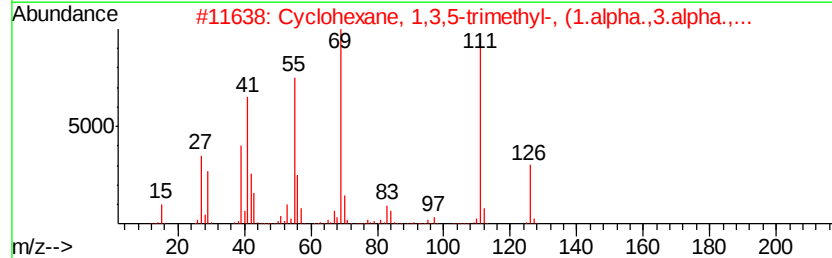
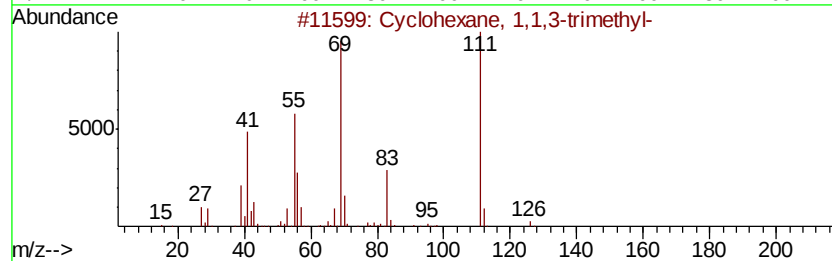
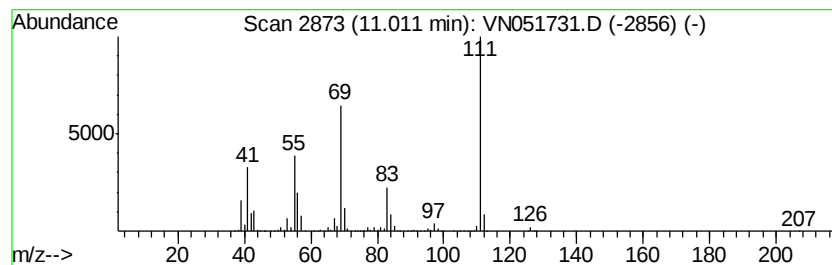
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N100418W.M
Quant Title : SW846 8260

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

Peak Number 1 Cyclohexane, 1,1,3-trimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.01	137.60 ug/l	7827310	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, 1,3,5-trimethyl-, (...	126	C9H18	001795-26-2	64
3		Cyclohexane, 1,3,5-trimethyl-	126	C9H18	001839-63-0	64
4		Cyclohexane, 1-ethyl-2,4-dimethyl-	140	C10H20	061142-69-6	64
5		Cyclohexane, 1,3,5-trimethyl-, (...	126	C9H18	001795-27-3	59



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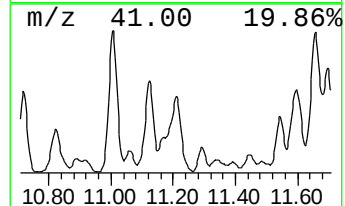
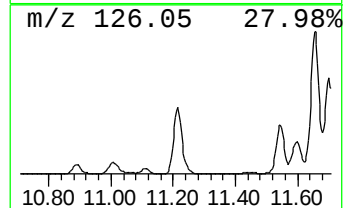
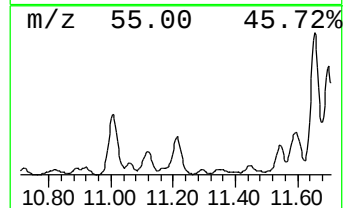
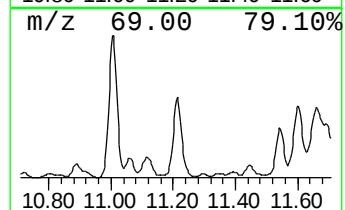
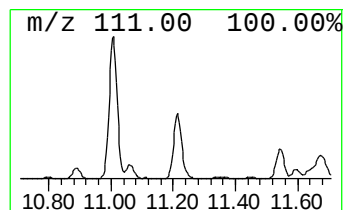
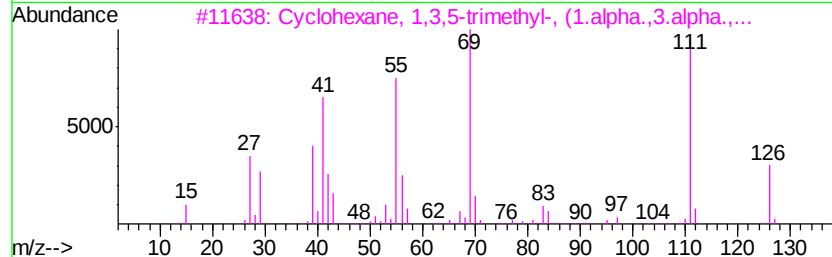
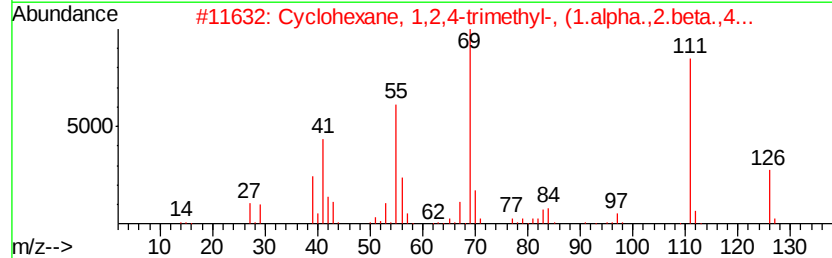
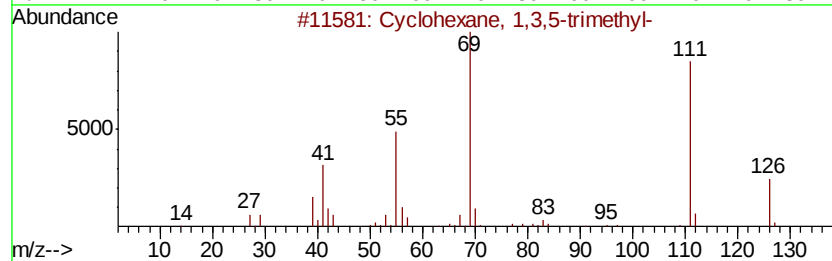
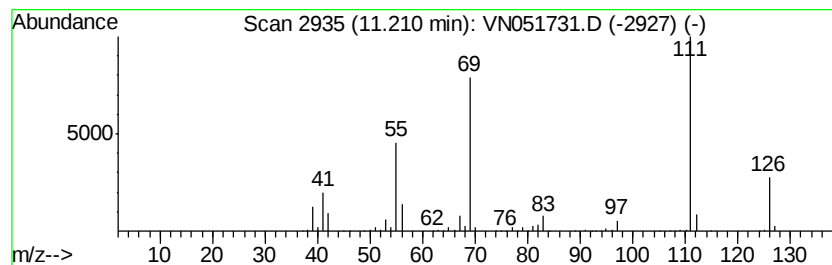
Instrument :
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Cyclohexane, 1,3,5-trimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.		
11.21	83.23 ug/l	4734870	Chlorobenzene-d5	11.41		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,3,5-trimethyl-	126	C9H18	001839-63-0	91	
2	Cyclohexane, 1,2,4-trimethyl-, (...	126	C9H18	007667-60-9	91	
3	Cyclohexane, 1,3,5-trimethyl-, (...	126	C9H18	001795-26-2	91	
4	Cyclohexane, 1,3,5-trimethyl-, (...	126	C9H18	001795-27-3	91	
5	2-Pyrazoline, 1-isopropyl-5-methyl-	126	C7H14N2	026964-54-5	72	



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Instrument :
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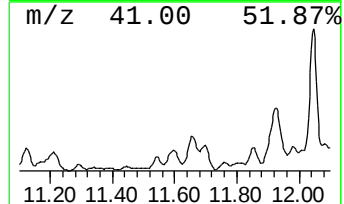
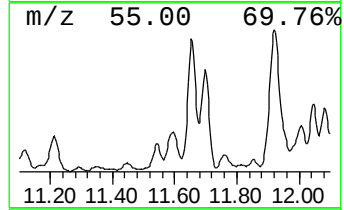
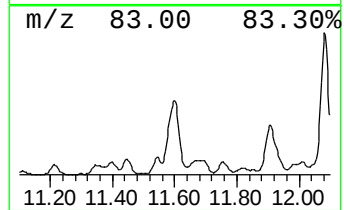
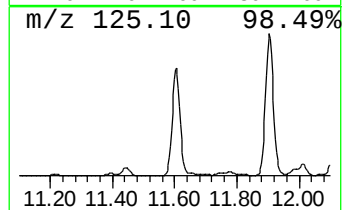
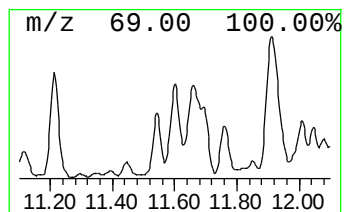
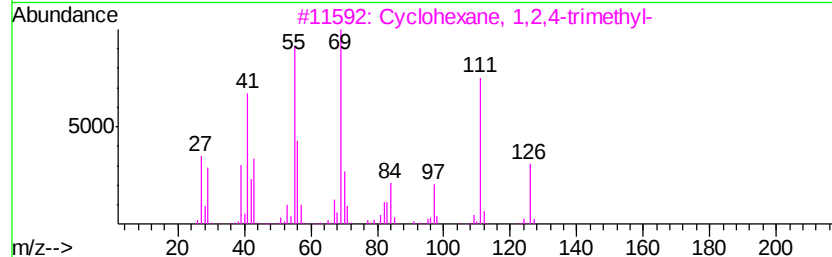
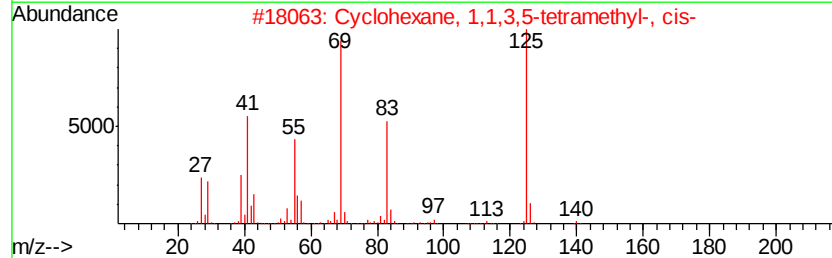
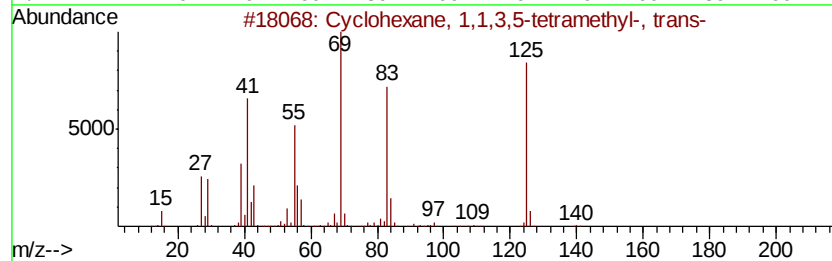
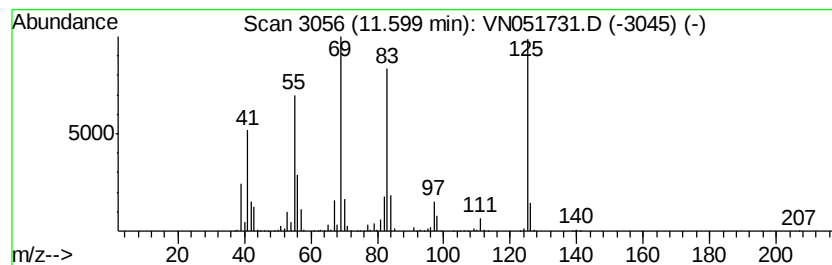
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Quant Title : SW846 8260

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

Peak Number 3 Cyclohexane, 1,1,3,5-tetram... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.60	78.42 ug/l	4460790	Chlorobenzene-d5	11.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, 1,1,3,5-tetramethyl...	140	C10H20	050876-31-8	68
2		Cyclohexane, 1,1,3,5-tetramethyl...	140	C10H20	050876-32-9	49
3		Cyclohexane, 1,2,4-trimethyl-	126	C9H18	002234-75-5	38
4		2,2-Dimethyl-3-heptene trans	126	C9H18	019550-75-5	30
5		Cyclohexane, 1,1,2-trimethyl-	126	C9H18	007094-26-0	25



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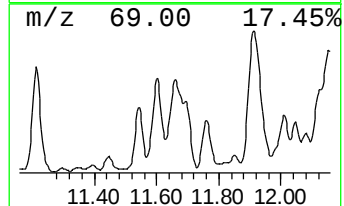
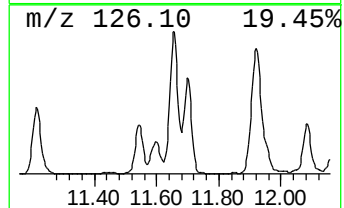
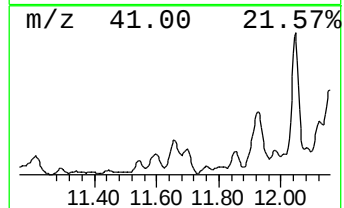
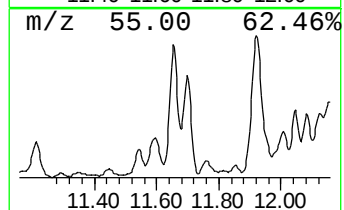
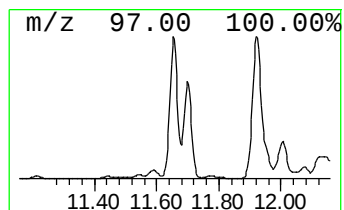
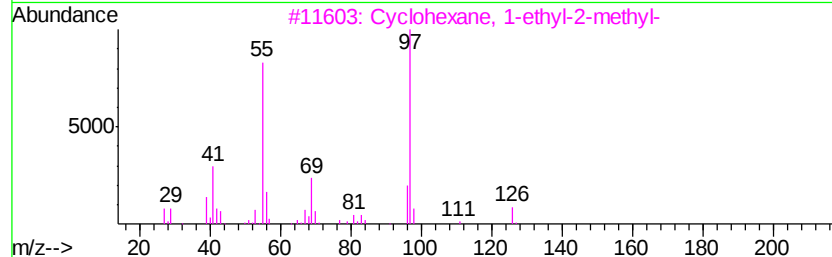
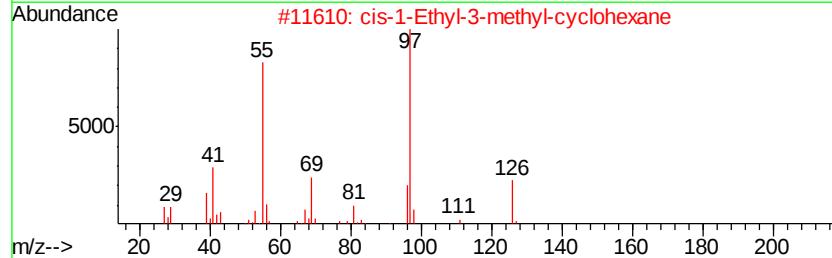
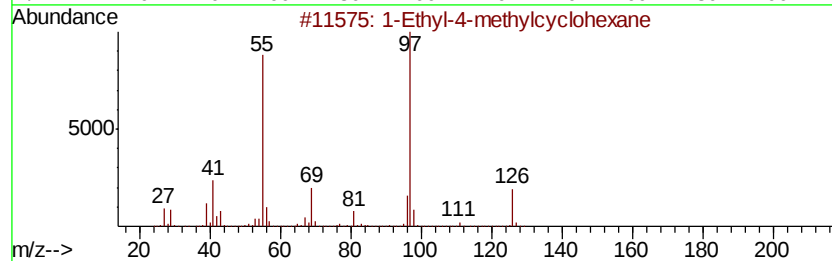
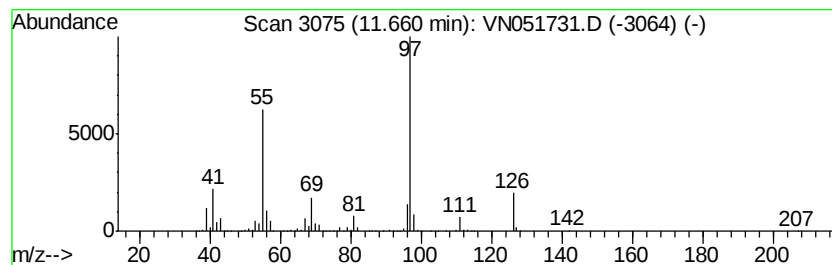
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.66	155.61 ug/l	8851950	Chlorobenzene-d5	11.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Ethyl-4-methylcyclohexane	126	C9H18	003728-56-1	94
2		cis-1-Ethyl-3-methyl-cyclohexane	126	C9H18	019489-10-2	91
3		Cyclohexane, 1-ethyl-2-methyl-	126	C9H18	003728-54-9	91
4		1-Ethyl-3-methylcyclohexane (c,t)	126	C9H18	003728-55-0	91
5		Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	004926-78-7	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN100818\
Data File : VN051731.D
Acq On : 8 Oct 2018 13:20
Operator : MD\SY
Sample : J5165-05 10X
Misc : 6.24g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 28

Instrument :
MSVOA_N
ClientSampleId :
EP1-MW-D-092718(7-10)

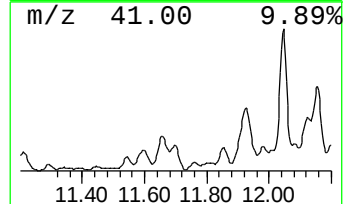
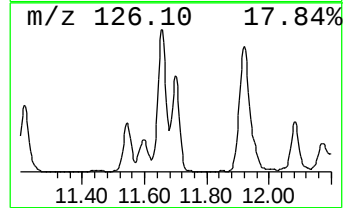
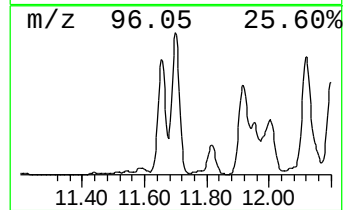
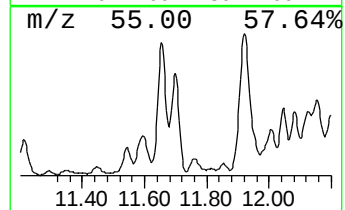
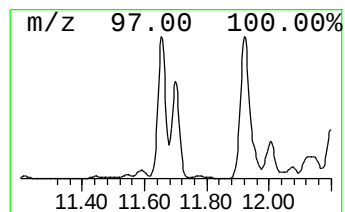
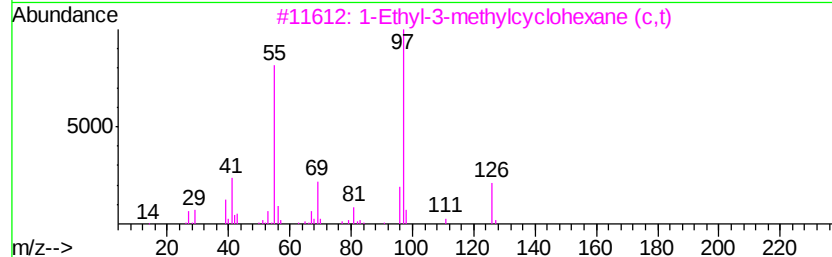
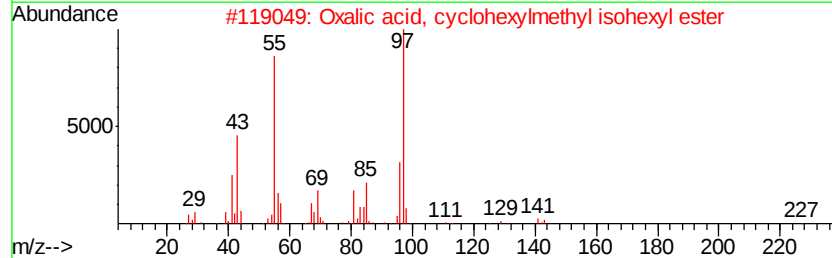
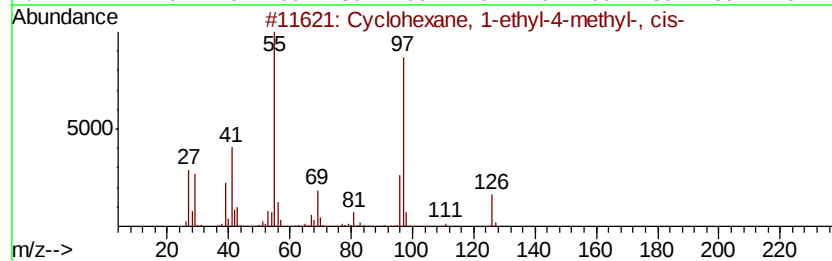
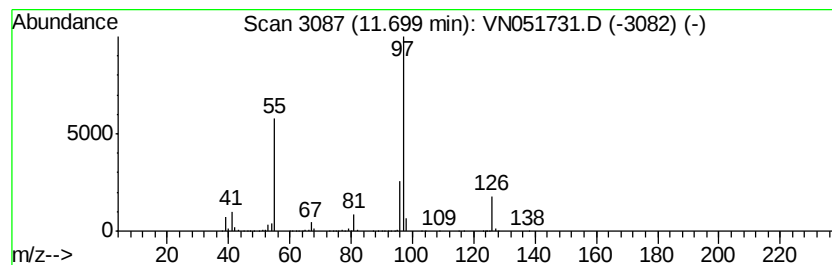
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Quant Title : SW846 8260

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

Peak Number 5 Cyclohexane, 1-ethyl-4-meth... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.70	98.66 ug/l	5612550	Chlorobenzene-d5	11.41

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	004926-78-7	83
2		Oxalic acid, cyclohexylmethyl is...	270	C15H26O4	1000309-68-3	78
3		1-Ethyl-3-methylcyclohexane (c,t)	126	C9H18	003728-55-0	72
4		Cyclohexane, 1-ethyl-1-methyl-	126	C9H18	004926-90-3	72
5		4-Octen-3-one	126	C8H14O	014129-48-7	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN100818\
Data File : VN051731.D
Acq On : 8 Oct 2018 13:20
Operator : MD\SY
Sample : J5165-05 10X
Misc : 6.24g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 28

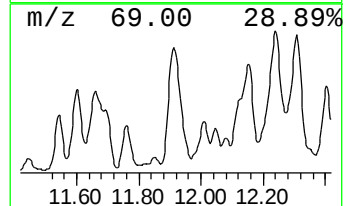
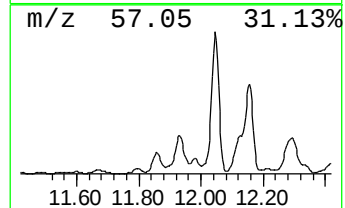
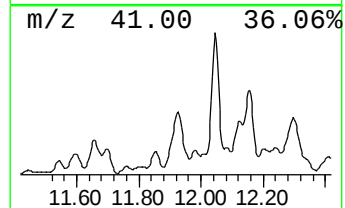
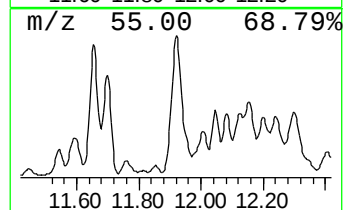
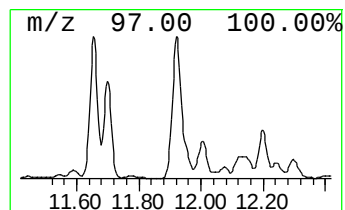
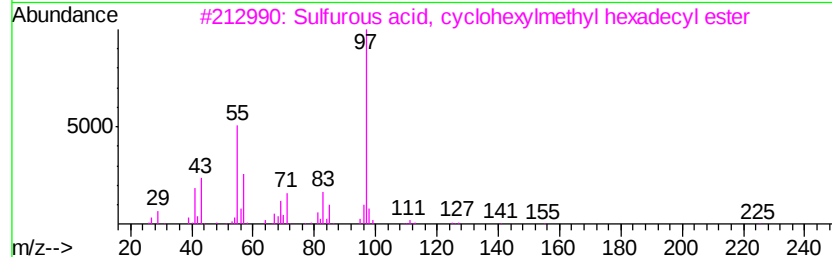
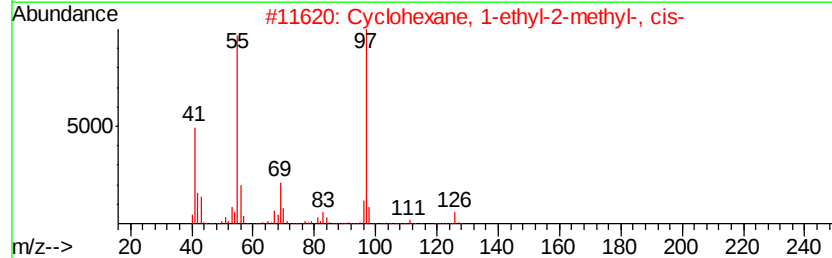
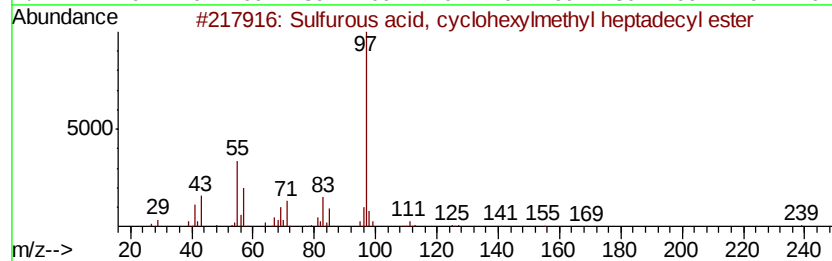
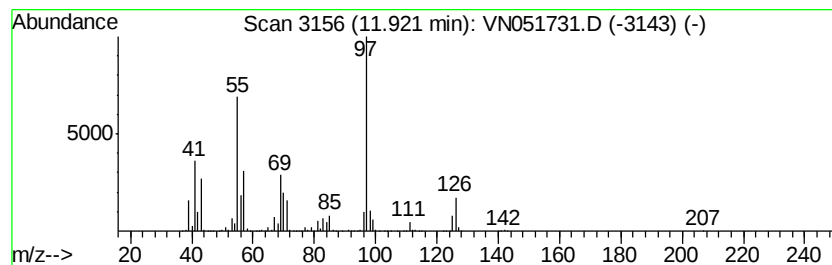
Instrument :
MSVOA_N
ClientSampleId :
EP1-MW-D-092718(7-10)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N100418W.M
Quant Title : SW846 8260

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

Peak Number 6 Sulfurous acid, cyclohexylm... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.		
11.92	305.51 ug/l	17379100	Chlorobenzene-d5	11.41		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Sulfurous acid, cyclohexylmethyl...	416	C24H48O3S	1000309-22-5	59
2		Cyclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-77-7	53
3		Sulfurous acid, cyclohexylmethyl...	402	C23H46O3S	1000309-22-4	53
4		Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	004926-78-7	52
5		Sulfurous acid, cyclohexylmethyl...	430	C25H50O3S	1000309-22-6	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN100818\
Data File : VN051731.D
Acq On : 8 Oct 2018 13:20
Operator : MD\SY
Sample : J5165-05 10X
Misc : 6.24g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 28

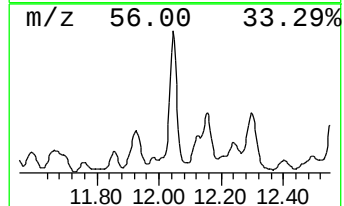
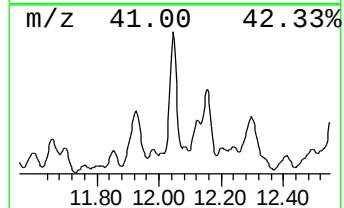
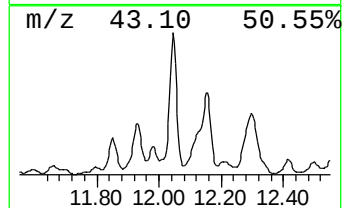
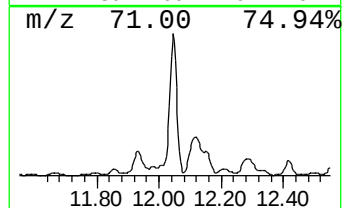
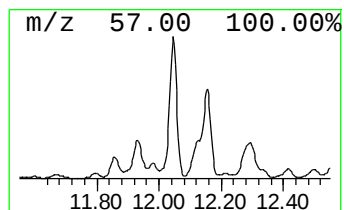
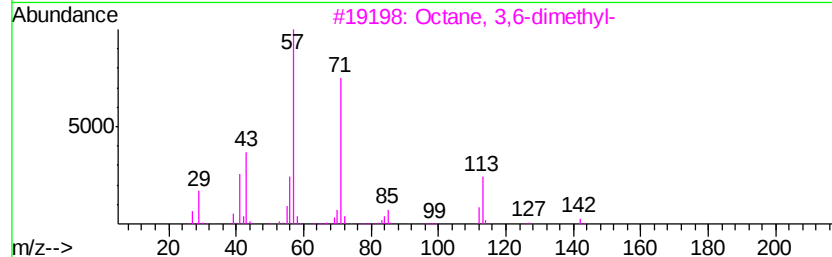
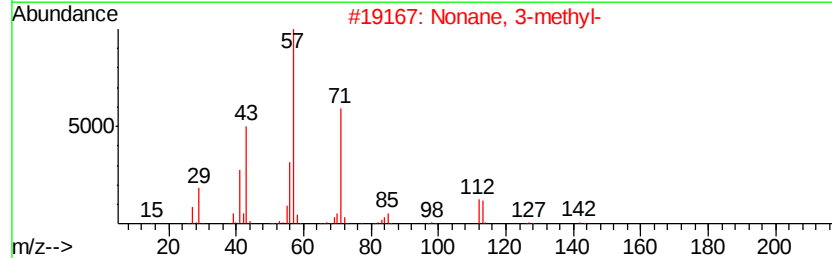
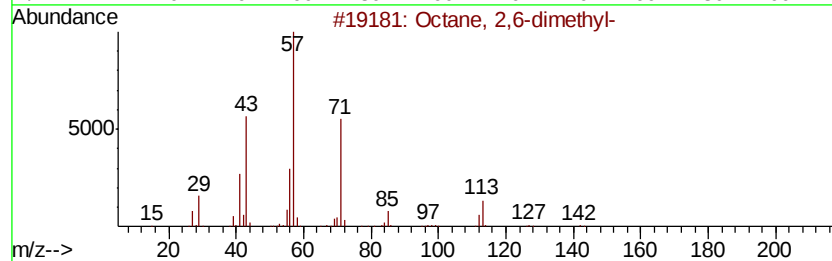
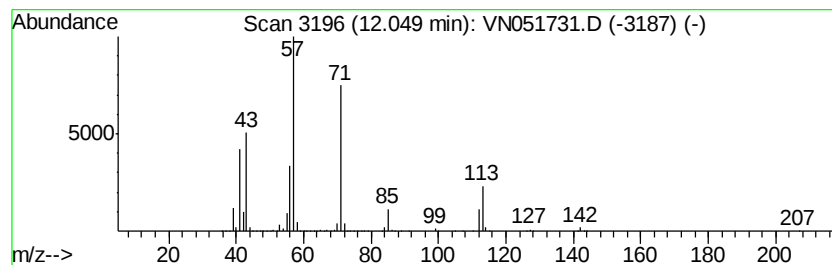
Instrument :
MSVOA_N
ClientSampleId :
EP1-MW-D-092718(7-10)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N100418W.M
Quant Title : SW846 8260

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

Peak Number 7 Octane, 2,6-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.		
12.05	257.47 ug/l	14646400	Chlorobenzene-d5	11.41		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	91	
2	Nonane, 3-methyl-	142	C10H22	005911-04-6	91	
3	Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	90	
4	Sulfurous acid, 2-ethylhexyl hex...	418	C24H50O3S	1000309-19-9	78	
5	Octane, 1,1'-oxybis-	242	C16H34O	000629-82-3	72	



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN100818\
Data File : VN051731.D
Acq On : 8 Oct 2018 13:20
Operator : MD\SY
Sample : J5165-05 10X
Misc : 6.24g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 28

Instrument :
MSVOA_N
ClientSampleId :
EP1-MW-D-092718(7-10)

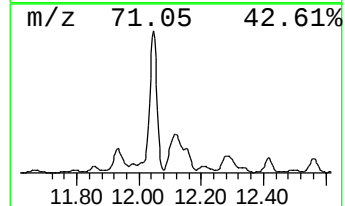
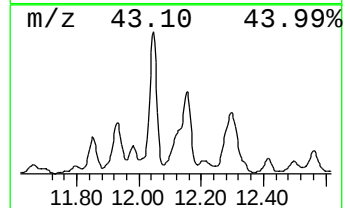
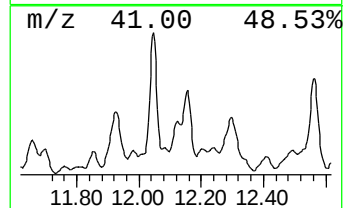
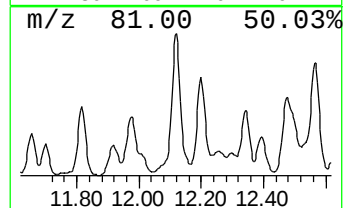
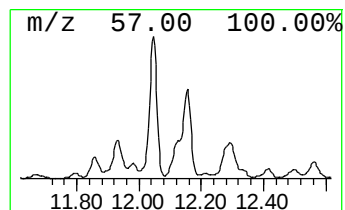
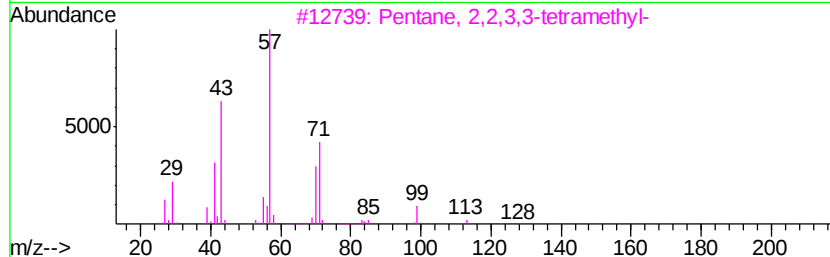
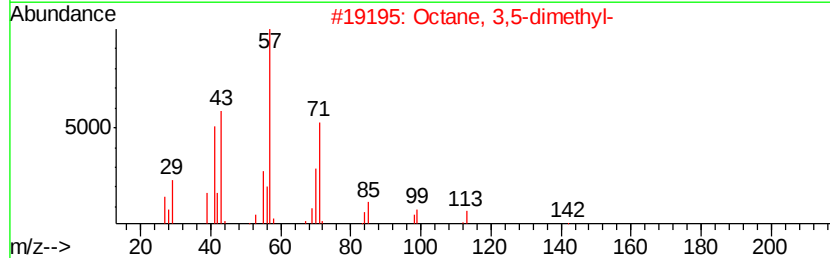
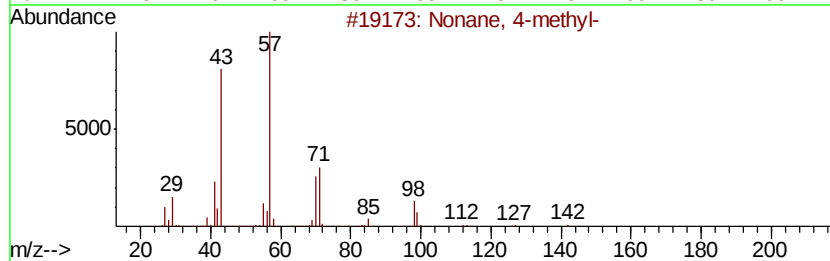
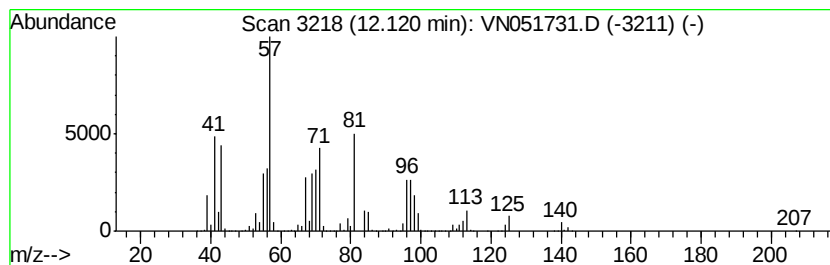
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Quant Title : SW846 8260

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

Peak Number 8 Nonane, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.12	104.74 ug/l	5958210	Chlorobenzene-d5	11.41

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonane, 4-methyl-	142	C10H22	017301-94-9	46	
2	Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	38	
3	Pentane, 2,2,3,3-tetramethyl-	128	C9H20	007154-79-2	35	
4	Decanal	156	C10H20O	000112-31-2	35	
5	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	27	



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN100818\
Data File : VN051731.D
Acq On : 8 Oct 2018 13:20
Operator : MD\SY
Sample : J5165-05 10X
Misc : 6.24g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 28

Instrument :
MSVOA_N
ClientSampleId :
EP1-MW-D-092718(7-10)

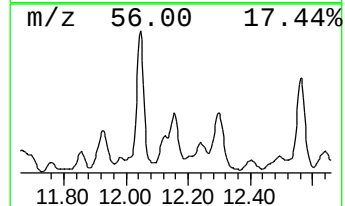
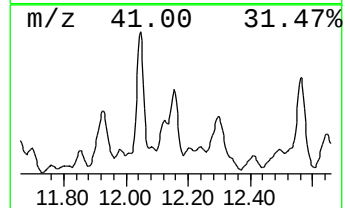
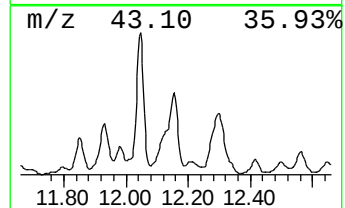
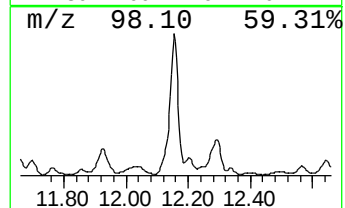
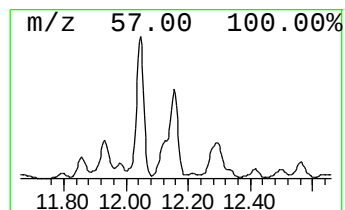
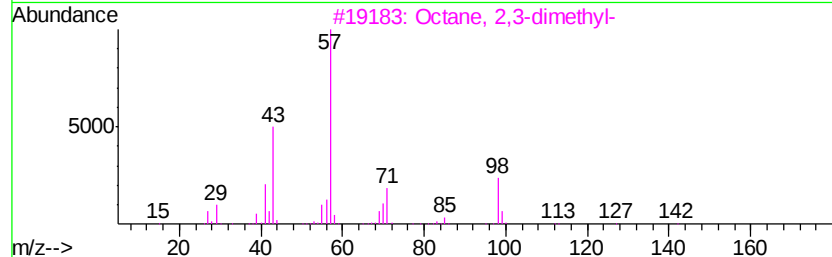
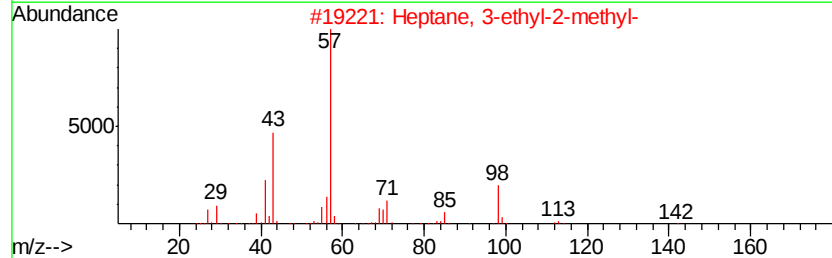
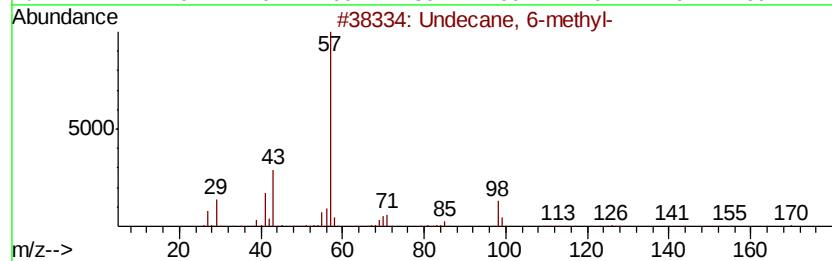
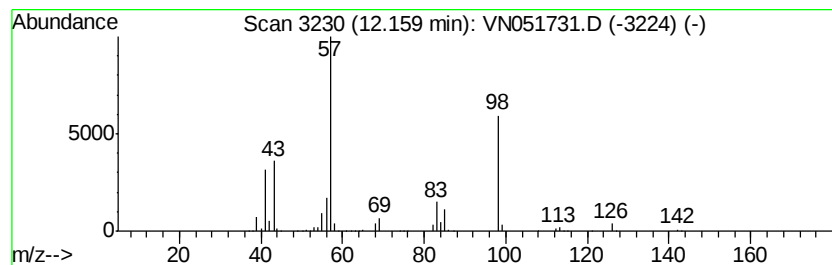
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Quant Title : SW846 8260

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

Peak Number 9 Undecane, 6-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.16	162.55 ug/l	9246760	Chlorobenzene-d5	11.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Undecane, 6-methyl-	170	C12H26	017302-33-9	53
2		Heptane, 3-ethyl-2-methyl-	142	C10H22	014676-29-0	50
3		Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	45
4		3H-Pyrazol-3-one, 2,4-dihydro-5-...	98	C4H6N2O	000108-26-9	43
5		1-Propene, 1,1'-oxybis-, (E,Z)-	98	C6H10O	004696-29-1	42



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN100818\
Data File : VN051731.D
Acq On : 8 Oct 2018 13:20
Operator : MD\SY
Sample : J5165-05 10X
Misc : 6.24g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 28

Instrument :
MSVOA_N
ClientSampleId :
EP1-MW-D-092718(7-10)

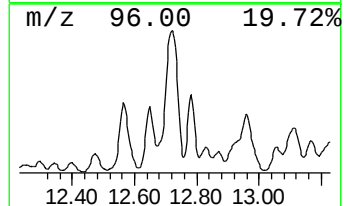
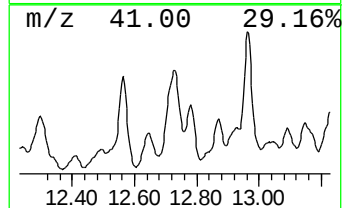
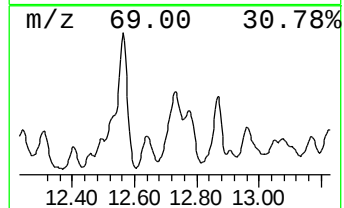
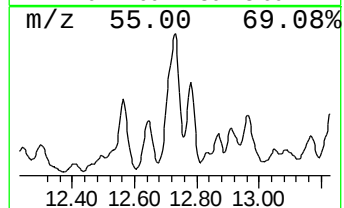
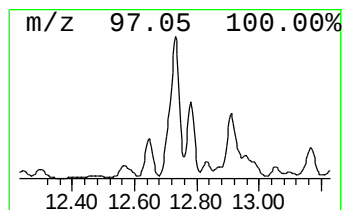
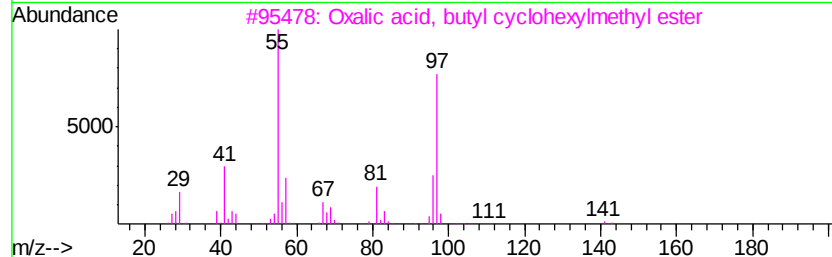
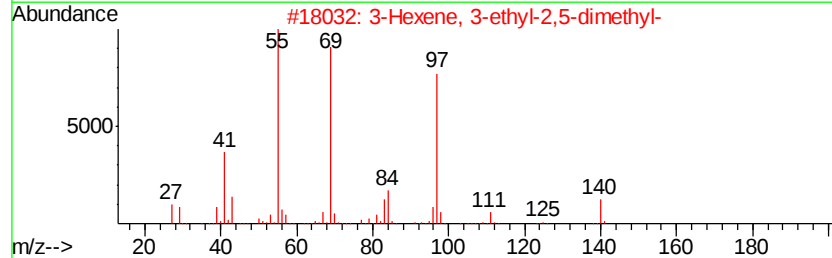
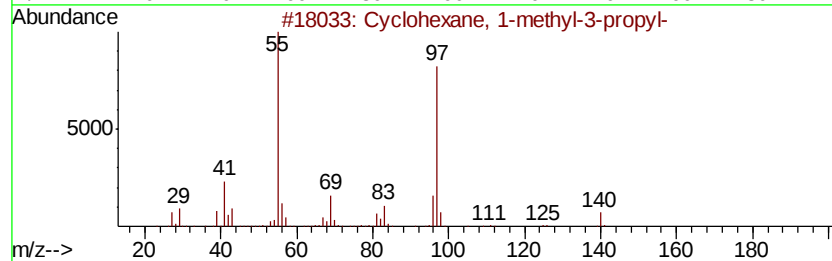
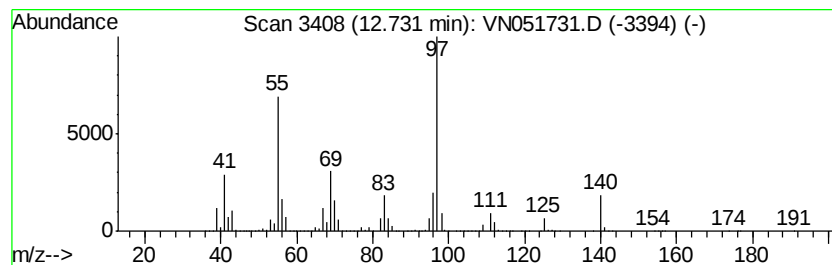
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Quant Title : SW846 8260

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

Peak Number 10 Cyclohexane, 1-methyl-3-pro... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.73	91.70 ug/l	37197500	1,4-Dichlorobenzene-d4	13.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, 1-methyl-3-propyl-	140	C10H20	004291-80-9	64
2		3-Hexene, 3-ethyl-2,5-dimethyl-	140	C10H20	062338-08-3	64
3		Oxalic acid, butyl cyclohexylmet...	242	C13H22O4	1000309-68-2	53
4		Cyclohexane, 1,1-dimethyl-	112	C8H16	000590-66-9	53
5		1-Ethyl-4-methylcyclohexane	126	C9H18	003728-56-1	52



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN100818\
Data File : VN051731.D
Acq On : 8 Oct 2018 13:20
Operator : MD\SY
Sample : J5165-05 10X
Misc : 6.24g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 28

Instrument :
MSVOA_N
ClientSampleId :
EP1-MW-D-092718(7-10)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N100418W.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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Cyclohexane, 1,3,...	11.21	83.2	ug/l	4734870	3	11.41	2844310	50.0
Cyclohexane, 1,1,...	11.60	78.4	ug/l	4460790	3	11.41	2844310	50.0
1-Ethyl-4-methylc...	11.66	155.6	ug/l	8851950	3	11.41	2844310	50.0
Cyclohexane, 1-et...	11.70	98.7	ug/l	5612550	3	11.41	2844310	50.0
Sulfurous acid, c...	11.92	305.5	ug/l	17379100	3	11.41	2844310	50.0
Octane, 2,6-dimet...	12.05	257.5	ug/l	14646400	3	11.41	2844310	50.0
Nonane, 4-methyl-	12.12	104.7	ug/l	5958210	3	11.41	2844310	50.0
Undecane, 6-methyl-	12.16	162.6	ug/l	9246760	3	11.41	2844310	50.0
Cyclohexane, 1-me...	12.73	91.7	ug/l	37197500	4	13.35	20281800	50.0