

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN101018\
 Data File : VN051789.D
 Acq On : 10 Oct 2018 14:30
 Operator : MD\SY
 Sample : J5165-20 10X
 Misc : 5.25g/5mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 14 Sample Multiplier: 28

Instrument :
 MSVOA_N
 ClientSampleId :
 EP1-MW-C(8-12)

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	1787	1810	1821	rBV3	589940	1487370	2.84%	0.296%
2	7.667	1821	1833	1852	rVB	959242	2277737	4.34%	0.453%
3	8.027	1927	1945	1968	rBV	554570	1290475	2.46%	0.256%
4	8.587	2103	2119	2145	rVB	1246126	2568865	4.90%	0.511%
5	9.082	2249	2273	2286	rBV2	248852	590620	1.13%	0.117%
6	10.091	2572	2587	2613	rBV2	2696245	5422478	10.34%	1.078%
7	10.432	2684	2693	2710	rVB	357805	668488	1.27%	0.133%
8	10.718	2771	2782	2794	rVB	643959	1082265	2.06%	0.215%
9	10.821	2794	2814	2826	rBV	489556	1072591	2.04%	0.213%
10	10.889	2826	2835	2843	rBV4	326974	605803	1.15%	0.120%
11	10.953	2846	2855	2862	rBV	971034	1444676	2.75%	0.287%
12	11.005	2862	2871	2882	rVB	1963558	3334248	6.36%	0.663%
13	11.124	2896	2908	2916	rBV3	1451979	2601953	4.96%	0.517%
14	11.210	2916	2935	2951	rVB5	2523443	7140989	13.61%	1.419%
15	11.294	2951	2961	2968	rBV	552482	922805	1.76%	0.183%
16	11.406	2984	2996	3014	rBV	1863644	4079142	7.78%	0.811%
17	11.490	3015	3022	3029	rBV4	332524	532815	1.02%	0.106%
18	11.545	3030	3039	3045	rBV	1694954	2741074	5.23%	0.545%
19	11.596	3045	3055	3063	rVV6	2417785	4744212	9.04%	0.943%
20	11.654	3064	3073	3081	rVV	8238617	15118988	28.82%	3.005%
21	11.699	3082	3087	3097	rVB2	5931369	8907131	16.98%	1.770%
22	11.760	3097	3106	3112	rBV3	1317294	2406200	4.59%	0.478%
23	11.853	3128	3135	3143	rVB3	3041678	4528090	8.63%	0.900%
24	11.924	3143	3157	3169	rBV5	12100389	29768405	56.75%	5.916%
25	12.046	3187	3195	3202	rBV	13991868	18784737	35.81%	3.733%
26	12.120	3210	3218	3224	rBV2	10777510	17641366	33.63%	3.506%
27	12.165	3224	3232	3250	rVB6	19721477	39099210	74.54%	7.771%
28	12.403	3296	3306	3316	rBV7	4906763	9653524	18.40%	1.919%
29	12.487	3317	3332	3339	rBV7	5333823	14990408	28.58%	2.979%
30	12.564	3348	3356	3372	rVB3	15610488	39296499	74.92%	7.810%
31	12.648	3372	3382	3391	rBV6	6986896	14570153	27.78%	2.896%
32	12.728	3394	3407	3416	rVV5	20397383	52451828	100.00%	10.424%
33	12.783	3417	3424	3434	rVB3	10502990	17471250	33.31%	3.472%
34	12.869	3444	3451	3458	rVV5	5333110	7336761	13.99%	1.458%

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Instrument :
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ClientSampleId :
EP1-MW-C(8-12)

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

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35	12.927	3459	3469	3472	rVV3	3865121	7771996	14.82%	1.545%
36	12.963	3473	3480	3494	rVB3	17996877	31214478	59.51%	6.204%
37	13.168	3533	3544	3552	rVV5	7099697	14344349	27.35%	2.851%
38	13.239	3553	3566	3587	rVB3	14155356	33586420	64.03%	6.675%
39	13.513	3647	3651	3669	rVB3	4978999	9909066	18.89%	1.969%
40	13.612	3670	3682	3688	rBV2	3657369	7348528	14.01%	1.460%
41	13.664	3689	3698	3708	rVB3	11620571	20303023	38.71%	4.035%
42	13.889	3760	3768	3778	rVB	8524165	13693959	26.11%	2.722%
43	13.992	3792	3800	3810	rVB5	4774623	7998265	15.25%	1.590%
44	14.178	3848	3858	3863	rBV5	3244455	6449530	12.30%	1.282%
45	14.294	3886	3894	3899	rBV2	1262992	1993737	3.80%	0.396%
46	14.332	3900	3906	3913	rVB2	1550303	2225254	4.24%	0.442%
47	14.525	3961	3966	3973	rVB3	423573	546636	1.04%	0.109%
48	14.583	3974	3984	3996	rVV3	3625329	6977979	13.30%	1.387%
49	14.648	3997	4004	4014	rVB2	919958	1515698	2.89%	0.301%
50	14.850	4062	4067	4074	rVB3	508831	661565	1.26%	0.131%

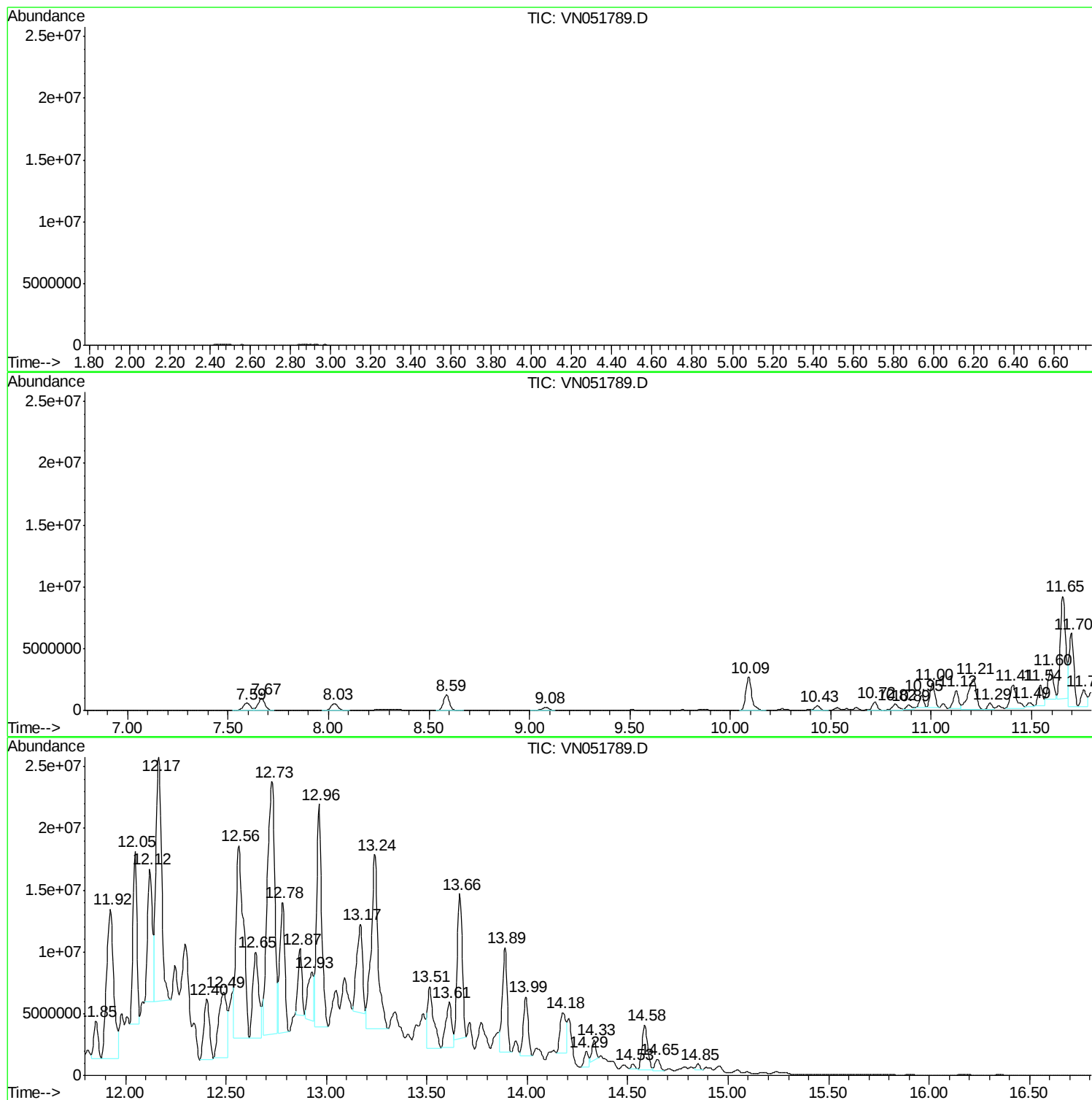
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N100418W.M
Quant Title : SW846 8260

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



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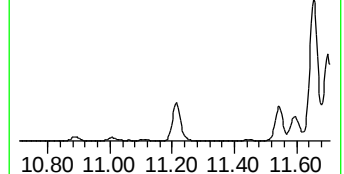
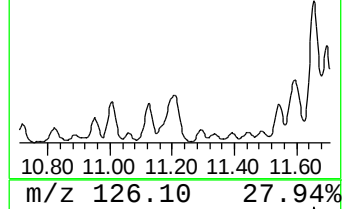
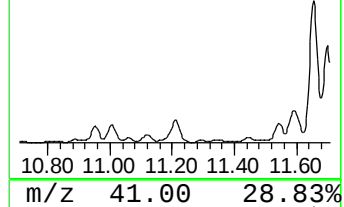
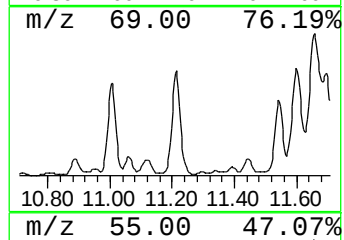
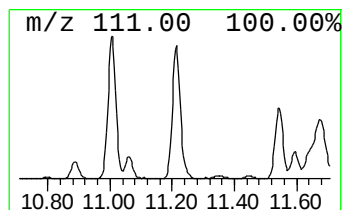
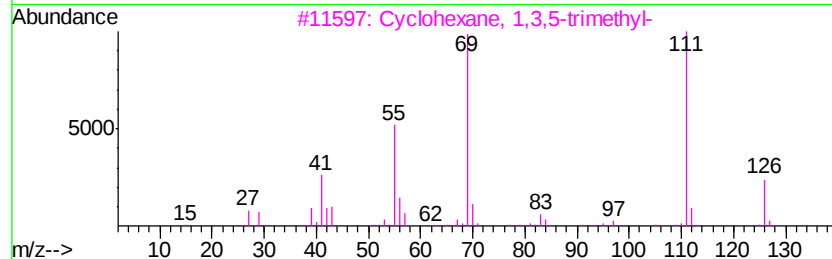
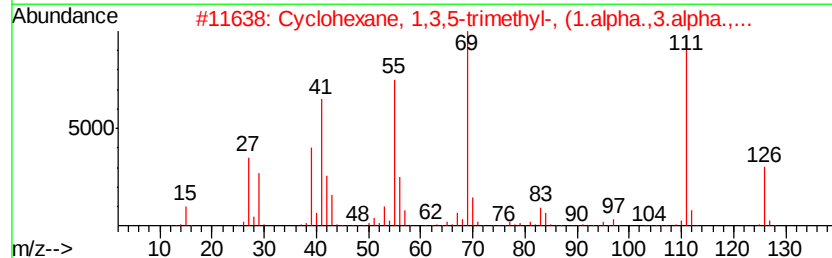
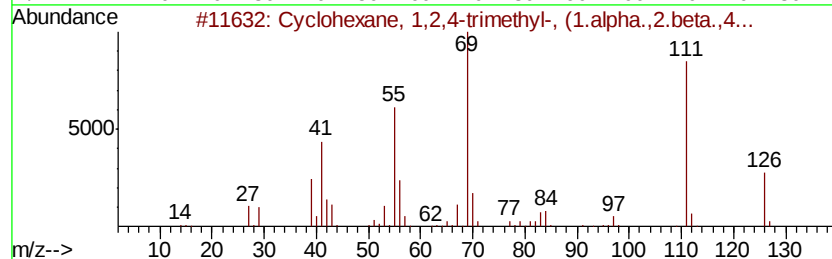
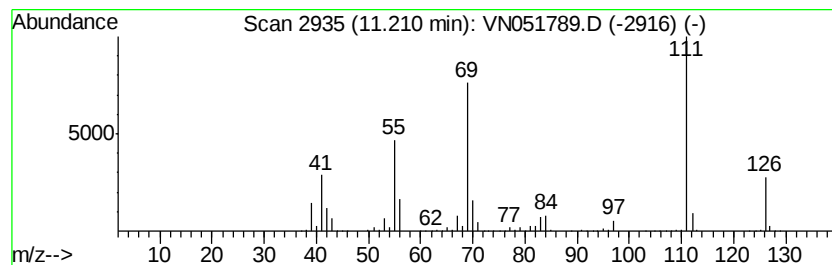
Instrument :
MSVOA_N
ClientSampleId :
EP1-MW-C(8-12)

Quant Method : Z:\V0ASRV\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, 1,2,4-trimethy... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.		
11.21	87.53 ug/l	7140990	Chlorobenzene-d5	11.41		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cvclohexane, 1,2,4-trimethyl-, (...	126	C9H18	007667-60-9	95
2		Cvclohexane, 1,3,5-trimethyl-, (...	126	C9H18	001795-26-2	91
3		Cvclohexane, 1,3,5-trimethyl-	126	C9H18	001839-63-0	91
4		Cvclohexane, 1,3,5-trimethyl-, (...	126	C9H18	001795-27-3	83
5		2-Pyrazoline, 1-isopropyl-5-methyl-	126	C7H14N2	026964-54-5	72



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ALS Vial : 14 Sample Multiplier: 28

Instrument :
MSVOA_N
ClientSampled :
EP1-MW-C(8-12)

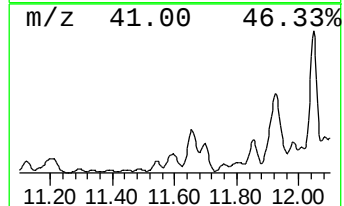
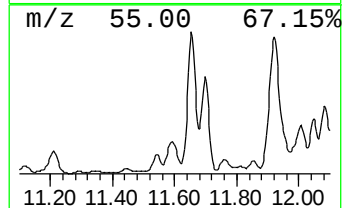
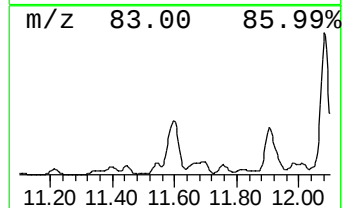
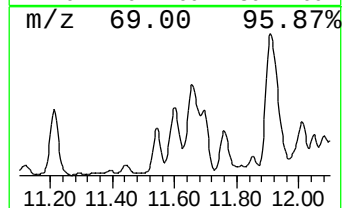
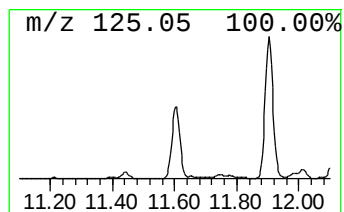
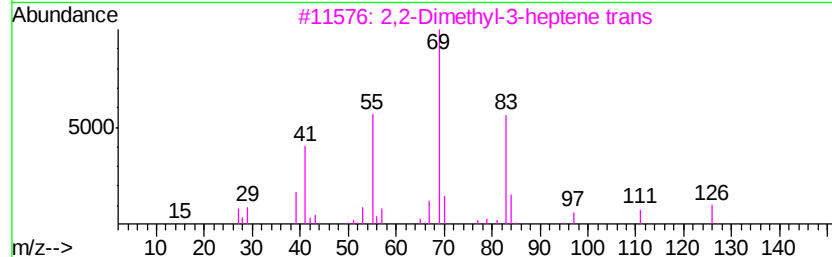
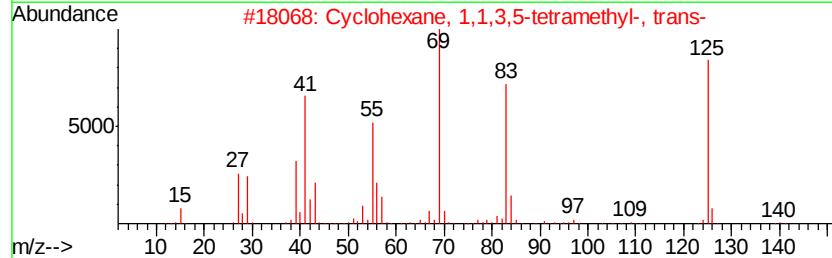
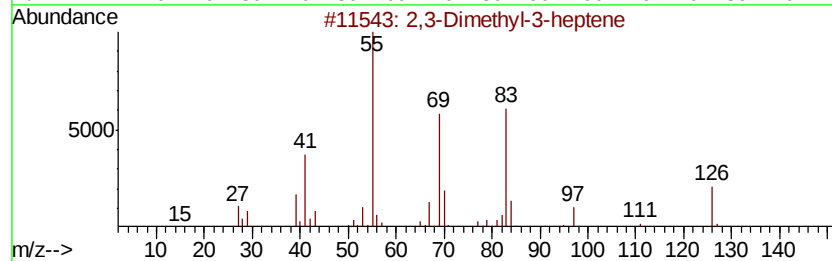
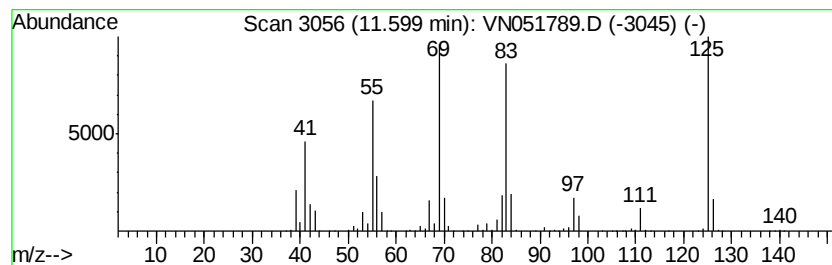
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N100418W.M
Quant Title : SW846 8260

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

Peak Number 2 2,3-Dimethyl-3-heptene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.60	58.15 ug/l	4744210	Chlorobenzene-d5	11.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2,3-Dimethyl-3-heptene	126	C9H18	1000113-49-3	58
2		Cyclohexane, 1,1,3,5-tetramethyl...	140	C10H20	050876-31-8	53
3		2,2-Dimethyl-3-heptene trans	126	C9H18	019550-75-5	38
4		Cyclohexane, 1,1,2-trimethyl-	126	C9H18	007094-26-0	30
5		1-Pentyn-3-ol, 3,4-dimethyl-	112	C7H12O	001482-15-1	22



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ALS Vial : 14 Sample Multiplier: 28

Instrument :
MSVOA_N
ClientSampleId :
EP1-MW-C(8-12)

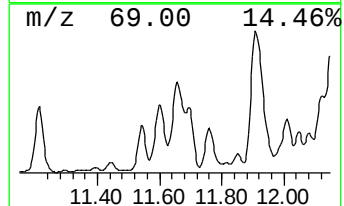
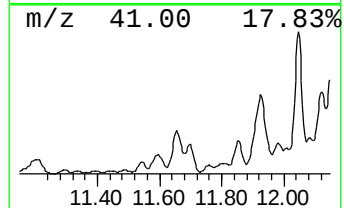
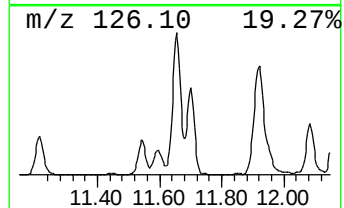
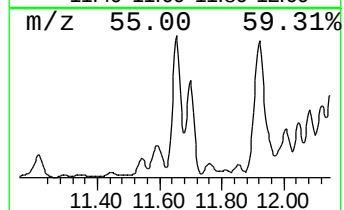
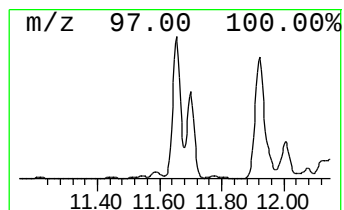
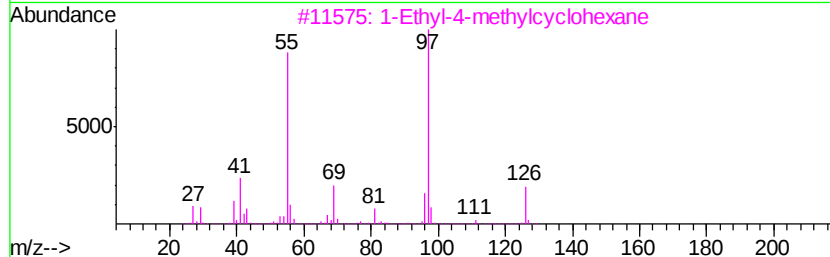
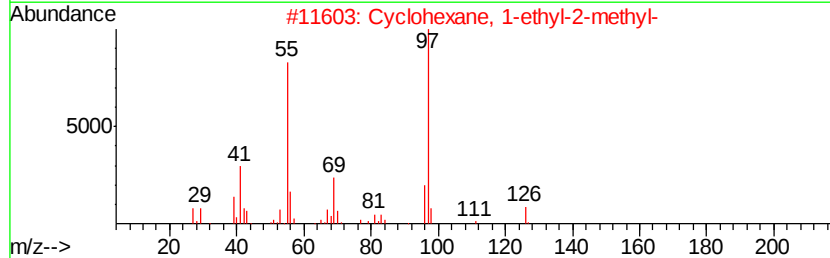
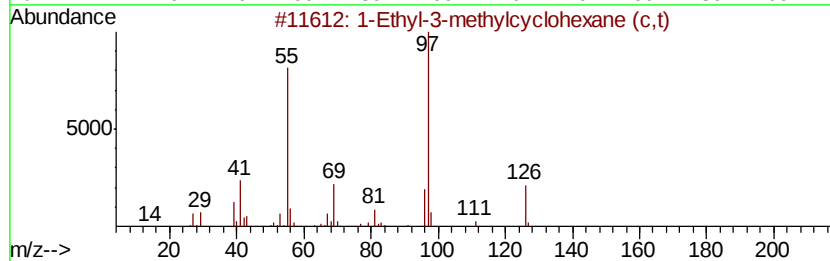
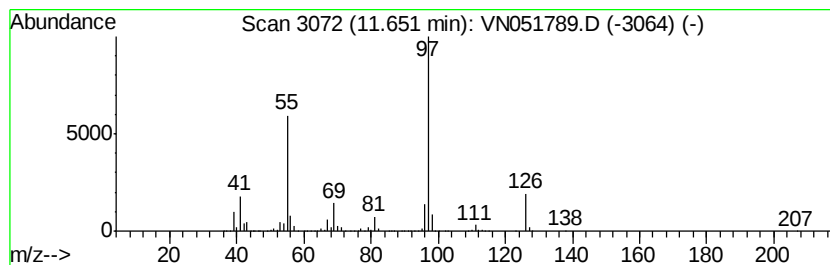
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Ethyl-3-methylcyclohexane... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.65	185.32 ug/l	15119000	Chlorobenzene-d5	11.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Ethyl-3-methylcyclohexane (c,t)	126	C9H18	003728-55-0	94
2		Cyclohexane, 1-ethyl-2-methyl-	126	C9H18	003728-54-9	91
3		1-Ethyl-4-methylcyclohexane	126	C9H18	003728-56-1	91
4		Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	004926-78-7	90
5		Cyclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-78-8	87



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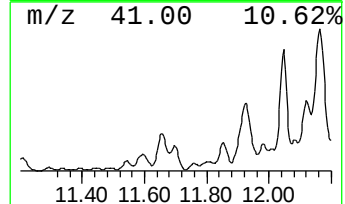
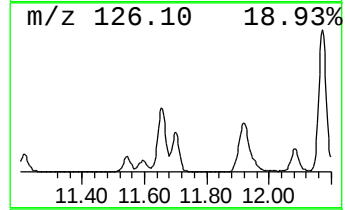
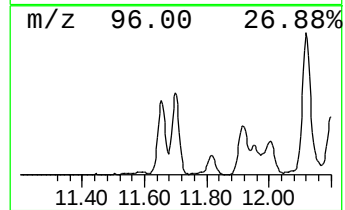
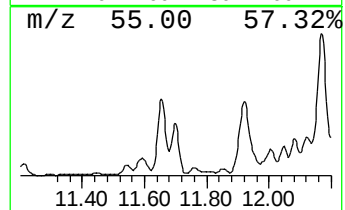
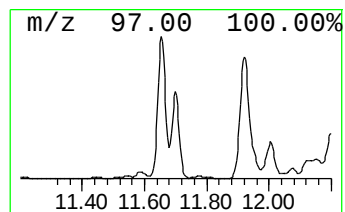
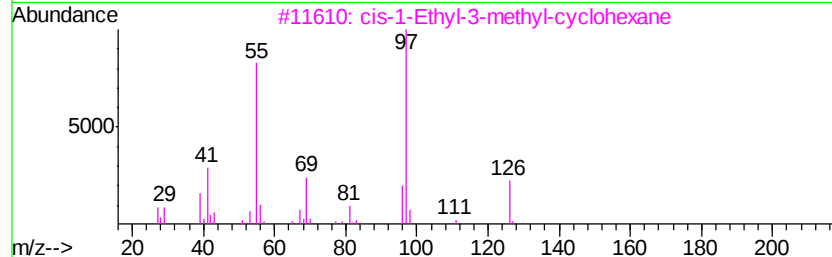
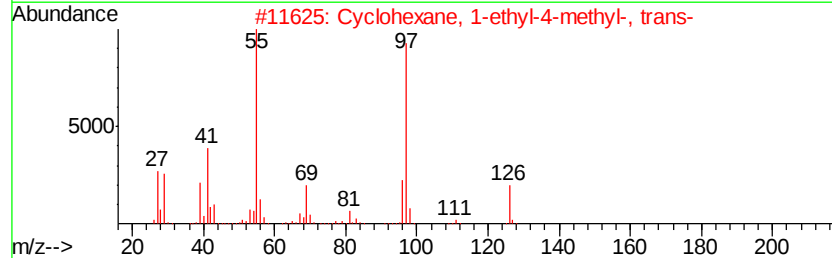
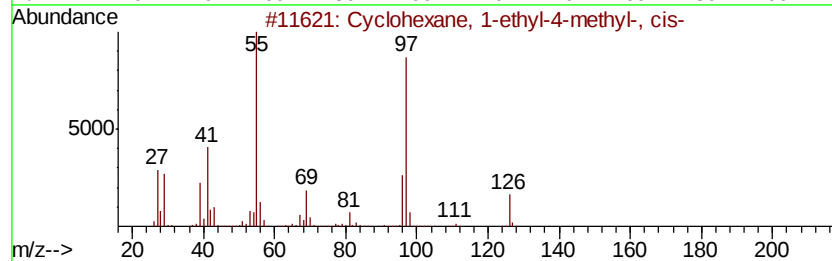
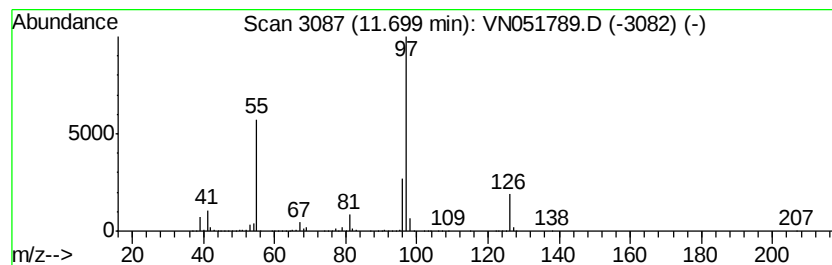
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Quant Title : SW846 8260

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

Peak Number 4 Cyclohexane, 1-ethyl-4-meth... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.70	109.18 ug/l	8907130	Chlorobenzene-d5	11.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	004926-78-7	83
2		Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	006236-88-0	78
3		cis-1-Ethyl-3-methyl-cyclohexane	126	C9H18	019489-10-2	78
4		Cyclohexane, 1-ethyl-1-methyl-	126	C9H18	004926-90-3	72
5		1-Ethyl-4-methylcyclohexane	126	C9H18	003728-56-1	64



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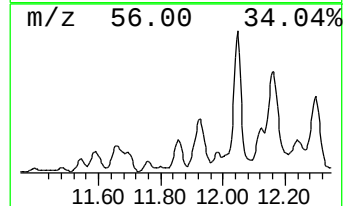
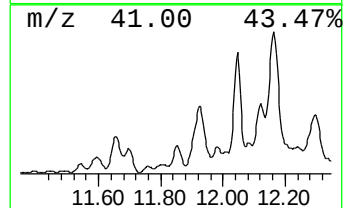
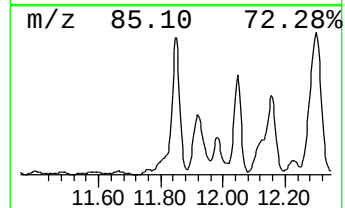
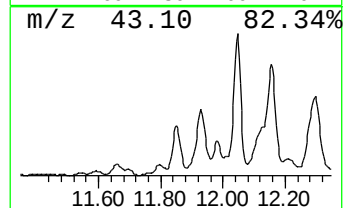
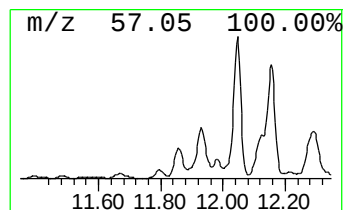
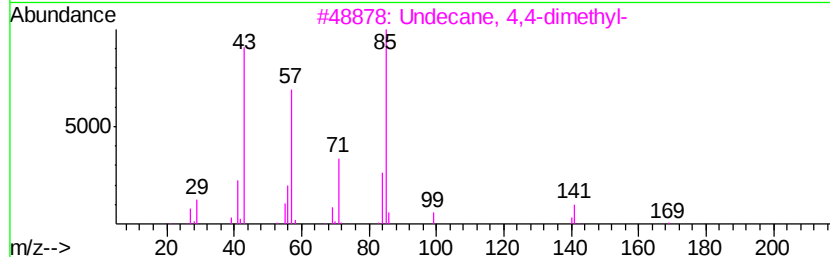
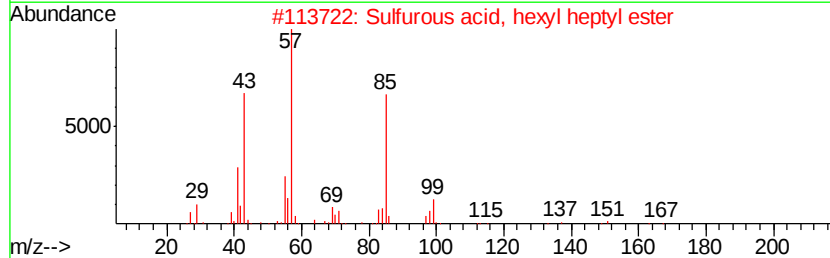
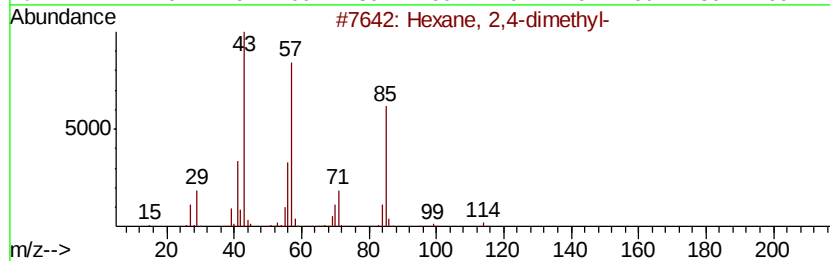
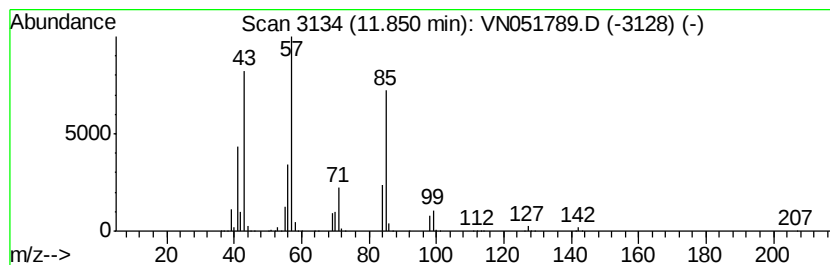
Instrument :
MSVOA_N
ClientSampleId :
EP1-MW-C(8-12)

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N100418W.M
Quant Title : SW846 8260

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

Peak Number 5 Hexane, 2,4-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.85	55.50 ug/l	4528090	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	Sulfurous acid, hexyl heptyl ester	264 C13H28O3S	1000309-12-9	53
3	Undecane, 4,4-dimethyl-	184 C13H28	017312-68-4	47
4	Heptane, 2,2,3,3,5,6,6-heptamethyl-	198 C14H30	007225-67-4	43
5	2,2-Dimethyl-3-heptanone	142 C9H18O	019078-97-8	43



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN101018\
Data File : VN051789.D
Acq On : 10 Oct 2018 14:30
Operator : MD\SY
Sample : J5165-20 10X
Misc : 5.25u/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 28

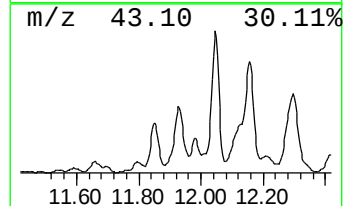
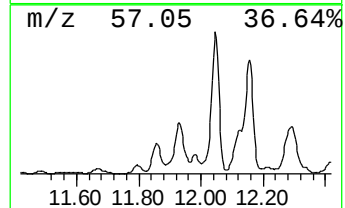
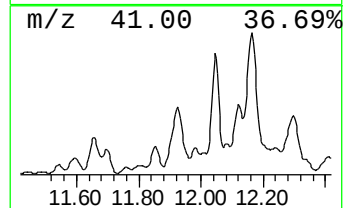
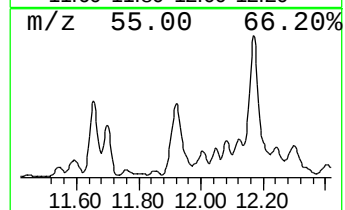
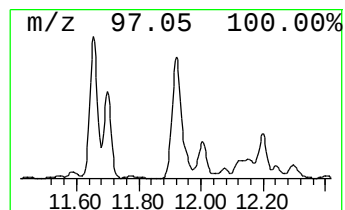
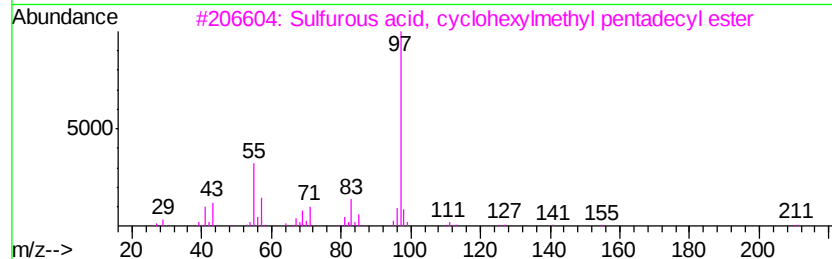
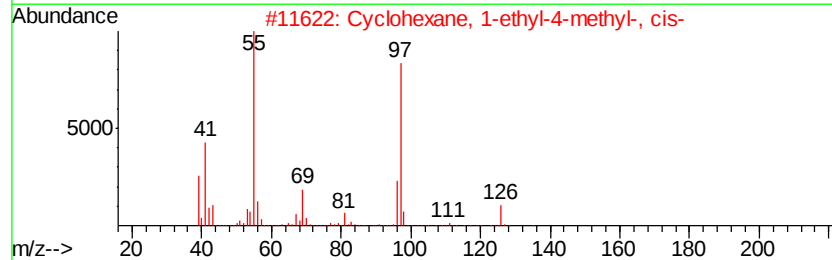
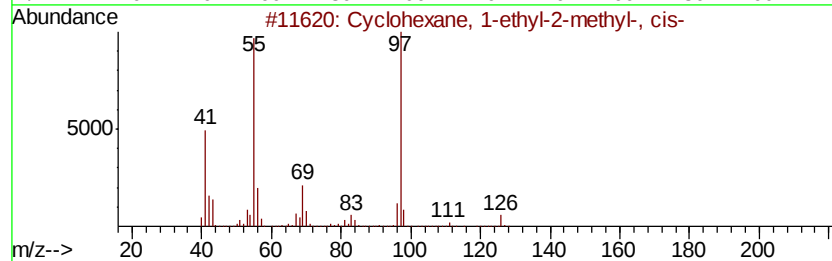
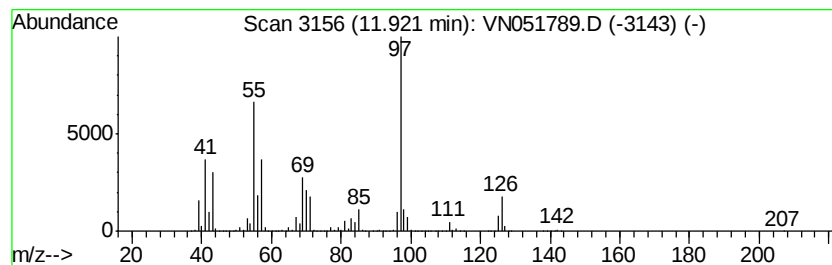
Instrument :
MSVOA_N
ClientSampleId :
EP1-MW-C(8-12)

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 Cyclohexane, 1-ethyl-2-meth... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.		
11.92	364.89 ug/l	29768400	Chlorobenzene-d5	11.41		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cvclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-77-7	53
2		Cvclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	004926-78-7	52
3		Sulfurous acid, cvclohexylmethyl...	388	C22H44O3S	1000309-22-3	50
4		Cvclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-78-8	49
5		3,5-Dimethyl-3-heptene	126	C9H18	059643-68-4	47



Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN101018\
 Data File : VN051789.D
 Acq On : 10 Oct 2018 14:30
 Operator : MD\SY
 Sample : J5165-20 10X
 Misc : 5.25a/5mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 14 Sample Multiplier: 28

Instrument :
 MSVOA_N
 ClientSampleId :
 EP1-MW-C(8-12)

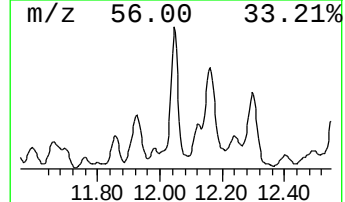
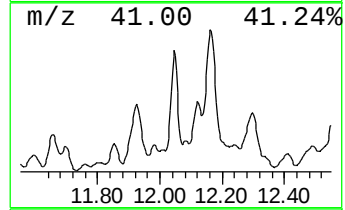
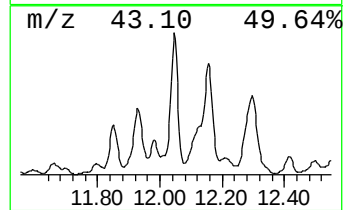
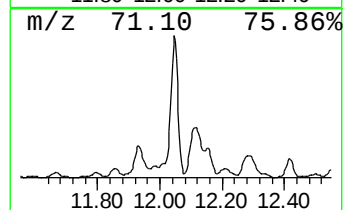
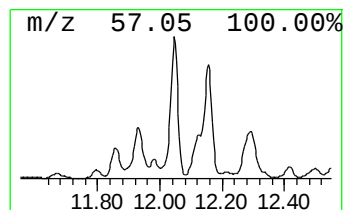
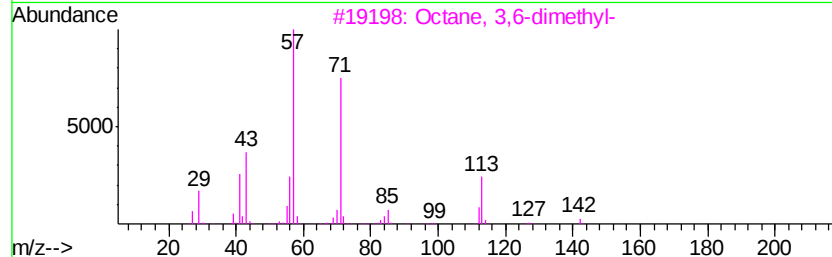
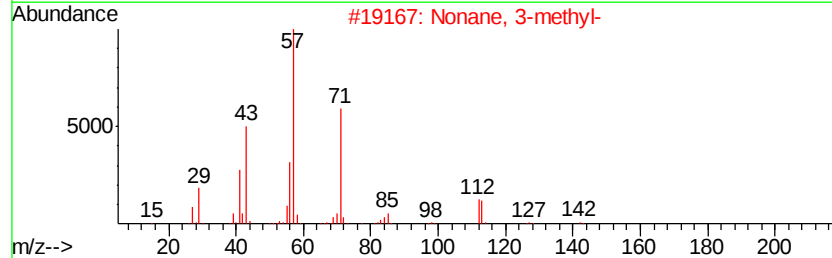
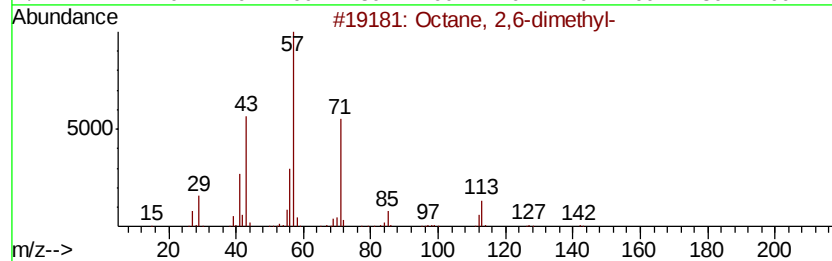
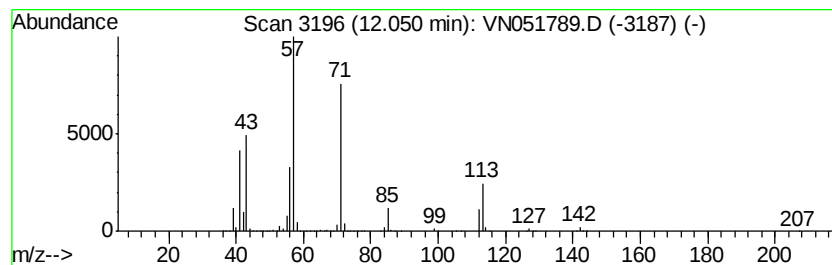
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 Quant Title : SW846 8260

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

 Peak Number 7 Octane, 2,6-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.05	230.25 ug/l	18784700	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	90
3		Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	80
4		Sulfurous acid, 2-ethylhexyl hep...	432	C25H52O3S	1000309-20-0	78
5		Octyl thioglycolate	204	C10H20O2S	007664-80-4	72



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN101018\
Data File : VN051789.D
Acq On : 10 Oct 2018 14:30
Operator : MD\SY
Sample : J5165-20 10X
Misc : 5.25g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 28

Instrument :
MSVOA_N
ClientSampleId :
EP1-MW-C(8-12)

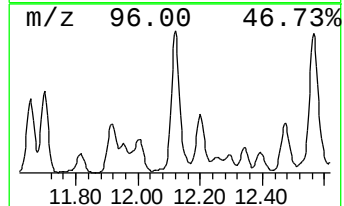
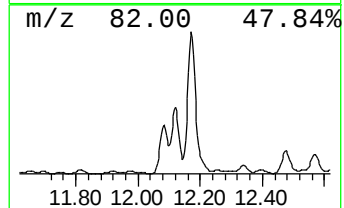
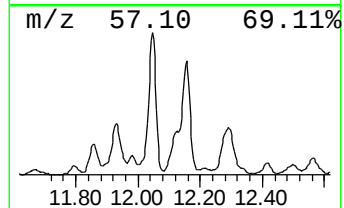
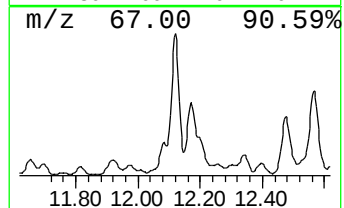
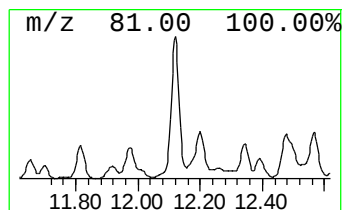
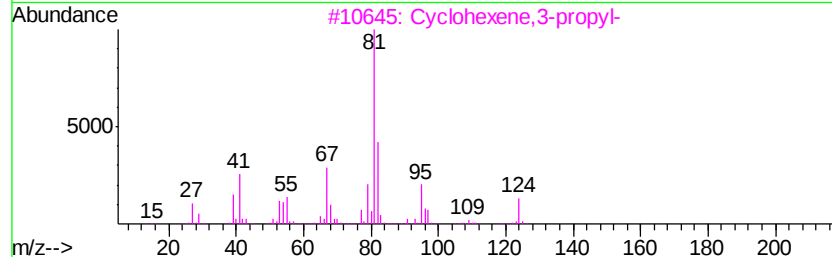
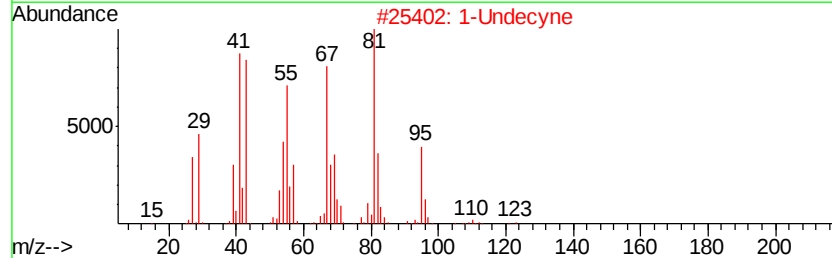
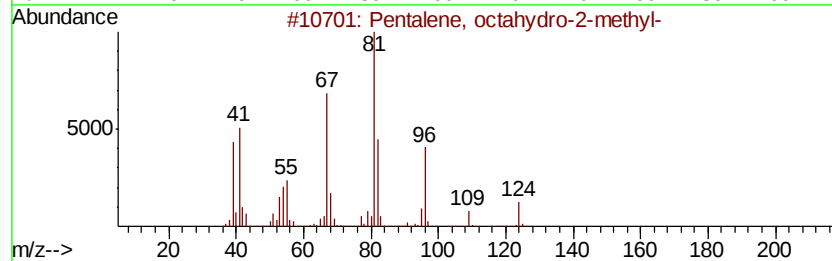
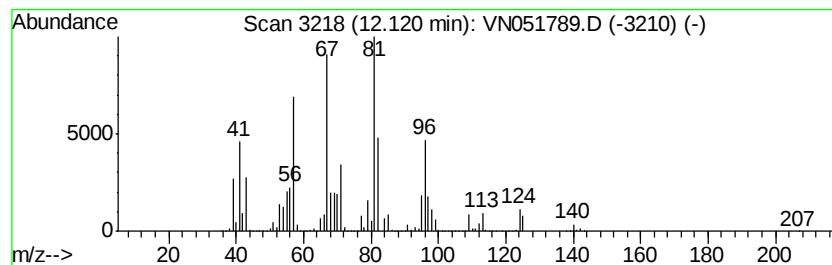
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Quant Title : SW846 8260

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

Peak Number 8 Pentalene, octahydro-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.12	216.24 ug/l	17641400	Chlorobenzene-d5	11.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentalene, octahydro-2-methyl-	124	C9H16	003868-64-2	90
2		1-Undecyne	152	C11H20	002243-98-3	53
3		Cyclohexene,3-propyl-	124	C9H16	003983-06-0	49
4		1H-Indene, octahydro-, trans-	124	C9H16	003296-50-2	49
5		Cyclohexene,3-butyl-	138	C10H18	003983-07-1	38



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA N\DATA\VN101018\
Data File : VN051789.D
Acq On : 10 Oct 2018 14:30
Operator : MD\SY
Sample : J5165-20 10X
Misc : 5.25g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 28

Instrument :
MSVOA_N
ClientSampleId :
EP1-MW-C(8-12)

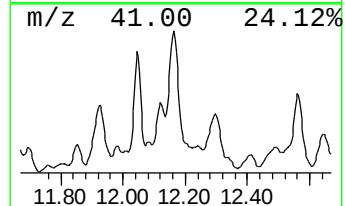
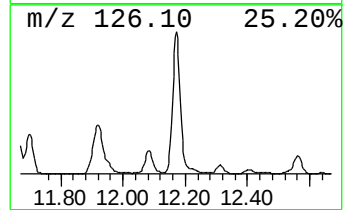
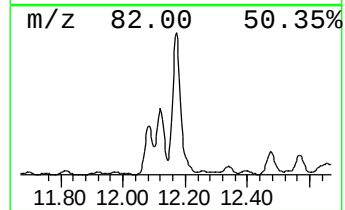
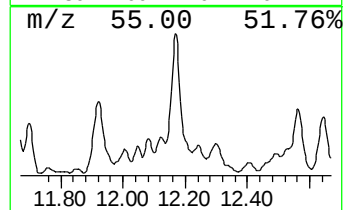
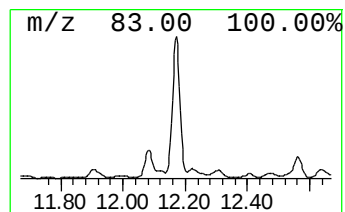
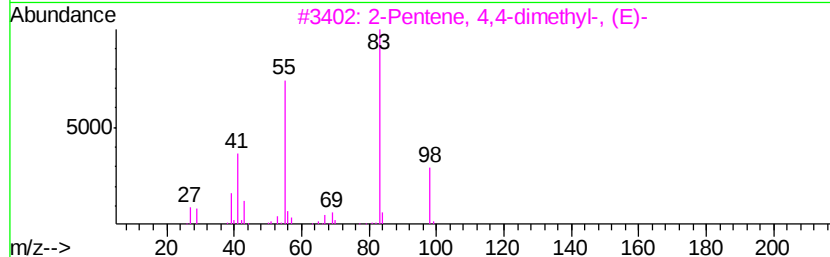
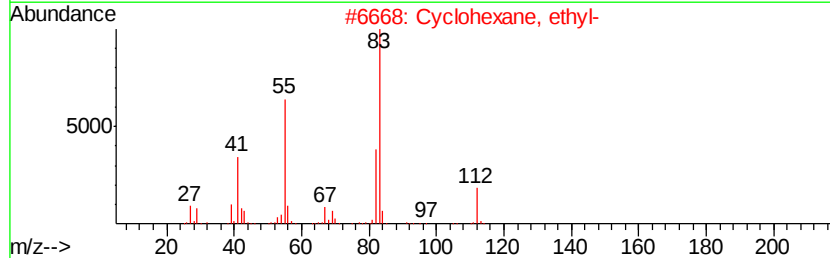
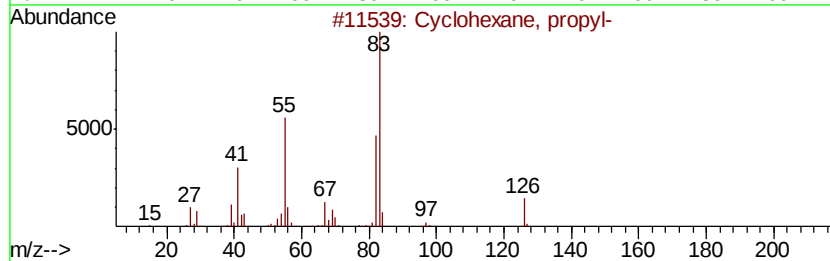
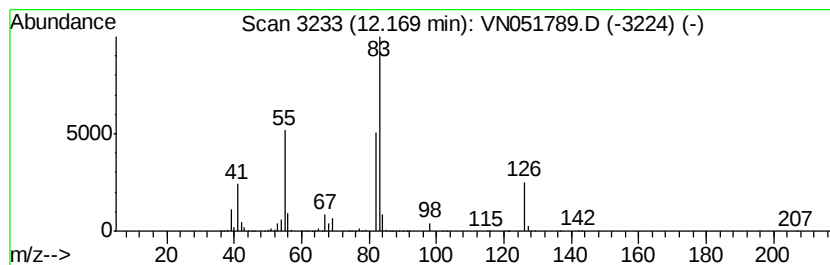
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Quant Title : SW846 8260

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

Peak Number 9 Cyclohexane, propyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.17	479.26 ug/l	39099200	Chlorobenzene-d5	11.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, propyl-	126	C9H18	001678-92-8	87
2		Cyclohexane, ethyl-	112	C8H16	001678-91-7	64
3		2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	52
4		Oxalic acid, cyclohexyl nonyl ester	298	C17H30O4	1000309-31-1	50
5		Oxalic acid, cyclohexyl dodecyl ...	340	C20H36O4	1000309-31-4	50



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_N\DATA\VN101018\
Data File : VN051789.D
Acq On : 10 Oct 2018 14:30
Operator : MD\SY
Sample : J5165-20 10X
Misc : 5.25g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 28

Instrument :
MSVOA_N
ClientSampleId :
EP1-MW-C(8-12)

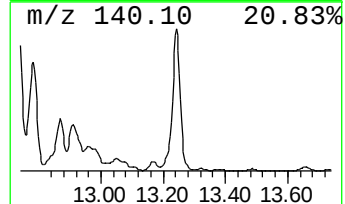
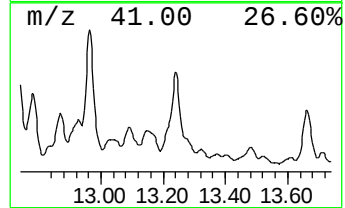
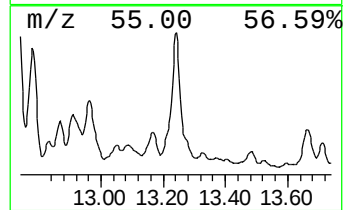
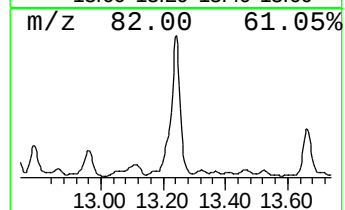
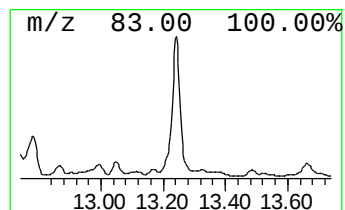
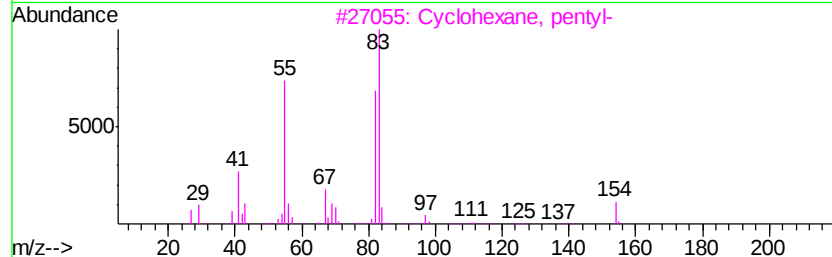
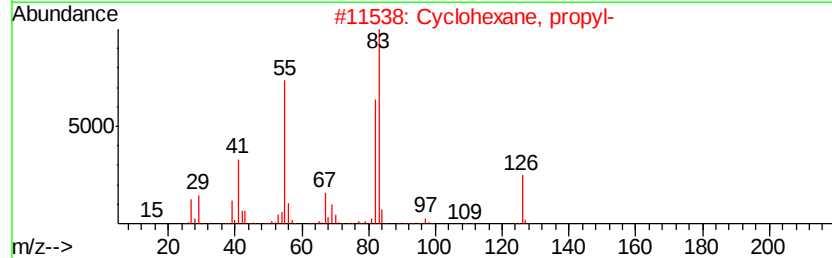
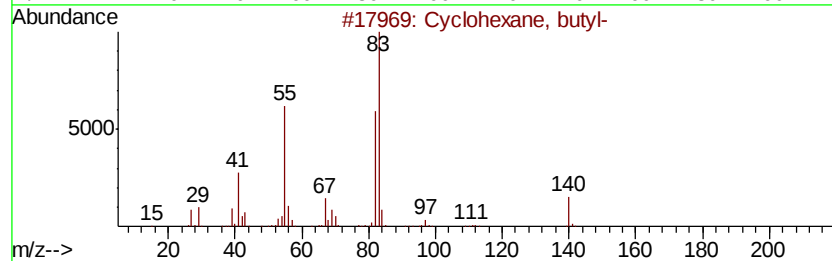
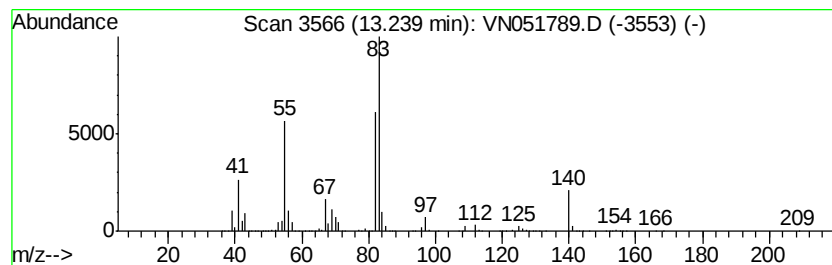
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N100418W.M
Quant Title : SW846 8260

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	33586400	1,4-Dichlorobenzene-d4	13.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, butyl-	140	C10H20	001678-93-9	95
2		Cyclohexane, propyl-	126	C9H18	001678-92-8	83
3		Cyclohexane, pentyl-	154	C11H22	004292-92-6	83
4		Cyclohexane, undecyl-	238	C17H34	054105-66-7	80
5		Cyclohexane, ethyl-	112	C8H16	001678-91-7	80



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN101018\
Data File : VN051789.D
Acq On : 10 Oct 2018 14:30
Operator : MD\SY
Sample : J5165-20 10X
Misc : 5.25g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 28

Instrument :
MSVOA_N
ClientSampleId :
EP1-MW-C(8-12)

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
Cyclohexane, 1,2,...	11.21	87.5	ug/l	7140990	3	11.41	4079140	50.0
2,3-Dimethyl-3-he...	11.60	58.1	ug/l	4744210	3	11.41	4079140	50.0
1-Ethyl-3-methylc...	11.65	185.3	ug/l	15119000	3	11.41	4079140	50.0
Cyclohexane, 1-et...	11.70	109.2	ug/l	8907130	3	11.41	4079140	50.0
Hexane, 2,4-dimet...	11.85	55.5	ug/l	4528090	3	11.41	4079140	50.0
Cyclohexane, 1-et...	11.92	364.9	ug/l	29768400	3	11.41	4079140	50.0
Octane, 2,6-dimet...	12.05	230.3	ug/l	18784700	3	11.41	4079140	50.0
Pentalene, octahy...	12.12	216.2	ug/l	17641400	3	11.41	4079140	50.0
Cyclohexane, propyl-	12.17	479.3	ug/l	39099200	3	11.41	4079140	50.0
Cyclohexane, butyl-	13.24	50.0	ug/l	33586400	4	13.35	33586400	50.0