

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN100818\
 Data File : VN051729.D
 Acq On : 8 Oct 2018 12:31
 Operator : MD\SY
 Sample : J5165-02
 Misc : 6.24g/5mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 12 Sample Multiplier: 28

Instrument :
 MSVOA_N
 ClientSampleId :
 EP1-MW-092718-FD-S

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	7.590	1789	1809	1821	rBV	478248	1212836	11.26%	1.103%
2	7.664	1821	1832	1853	rVB	734373	1716263	15.93%	1.561%
3	8.027	1928	1945	1965	rBV	461849	1080372	10.03%	0.983%
4	8.252	1985	2015	2018	rBV3	53476	213443	1.98%	0.194%
5	8.587	2103	2119	2140	rBV	1001222	2058596	19.11%	1.873%
6	10.091	2566	2587	2617	rBV	1821673	3436889	31.90%	3.126%
7	10.718	2771	2782	2796	rVB	166580	278776	2.59%	0.254%
8	10.821	2799	2814	2827	rBV	96457	214513	1.99%	0.195%
9	11.005	2857	2871	2881	rBV2	308192	596460	5.54%	0.543%
10	11.124	2896	2908	2916	rBV5	228742	424126	3.94%	0.386%
11	11.210	2916	2935	2951	rVB6	336348	1024548	9.51%	0.932%
12	11.297	2951	2962	2972	rBV	340432	597611	5.55%	0.544%
13	11.406	2983	2996	3015	rBV	1415530	2630600	24.42%	2.393%
14	11.542	3029	3038	3045	rBV	207099	339010	3.15%	0.308%
15	11.596	3045	3055	3064	rVV6	313888	644131	5.98%	0.586%
16	11.654	3064	3073	3080	rVV	587760	1123056	10.43%	1.022%
17	11.699	3082	3087	3097	rVB	571951	873591	8.11%	0.795%
18	11.760	3097	3106	3111	rBV2	185138	321607	2.99%	0.293%
19	11.850	3127	3134	3143	rVB3	472734	725229	6.73%	0.660%
20	11.924	3143	3157	3168	rBV6	1501208	3551875	32.97%	3.231%
21	11.979	3170	3174	3179	rVV3	224870	245536	2.28%	0.223%
22	12.043	3186	3194	3203	rVB	2708427	3824668	35.50%	3.479%
23	12.120	3210	3218	3222	rBV4	901725	1455669	13.51%	1.324%
24	12.152	3223	3228	3238	rVB3	1814565	2876828	26.71%	2.617%
25	12.297	3264	3273	3279	rBV7	1107083	2023119	18.78%	1.840%
26	12.336	3280	3285	3294	rVB	2433980	3539307	32.86%	3.219%
27	12.403	3294	3306	3317	rVB5	1974354	3920615	36.40%	3.566%
28	12.493	3317	3334	3340	rBV8	817764	2206119	20.48%	2.007%
29	12.561	3348	3355	3371	rVB3	2581898	5426602	50.38%	4.936%
30	12.644	3371	3381	3391	rBV7	1207211	2690151	24.97%	2.447%
31	12.728	3393	3407	3416	rBV5	3245167	8123209	75.41%	7.389%
32	12.869	3444	3451	3458	rBV5	1289989	1987098	18.45%	1.808%
33	12.963	3473	3480	3493	rVB	6782686	10772272	100.00%	9.799%
34	13.040	3495	3504	3512	rVB2	2329276	3888748	36.10%	3.537%

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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	13.091	3513	3520	3529	rBV3	1195227	1801291	16.72%	1.639%
36	13.146	3531	3537	3541	rBV3	1210739	1743438	16.18%	1.586%
37	13.239	3552	3566	3573	rBV5	2658192	5223846	48.49%	4.752%
38	13.342	3593	3598	3608	rVB	1672991	2563440	23.80%	2.332%
39	13.612	3671	3682	3688	rBV2	636773	1448489	13.45%	1.318%
40	13.664	3689	3698	3707	rVV5	2766675	5284848	49.06%	4.807%
41	13.712	3709	3713	3721	rVB2	926708	1241668	11.53%	1.129%
42	13.834	3746	3751	3761	rVB5	1331945	1904966	17.68%	1.733%
43	13.886	3762	3767	3776	rVB2	1466739	2241517	20.81%	2.039%
44	13.934	3778	3782	3791	rVB2	717621	992521	9.21%	0.903%
45	13.992	3792	3800	3810	rVB4	952654	1696795	15.75%	1.543%
46	14.178	3848	3858	3865	rBV6	1138660	2355486	21.87%	2.143%
47	14.249	3874	3880	3888	rVB	1065957	1482996	13.77%	1.349%
48	14.294	3889	3894	3900	rVV4	368989	490624	4.55%	0.446%
49	14.332	3901	3906	3913	rVB4	478318	604906	5.62%	0.550%
50	14.525	3960	3966	3974	rVB2	370137	510612	4.74%	0.464%
51	14.590	3976	3986	3996	rVV4	638920	1396084	12.96%	1.270%
52	14.644	3996	4003	4015	rVB3	437467	778514	7.23%	0.708%
53	14.850	4062	4067	4073	rBV3	112110	129715	1.20%	0.118%

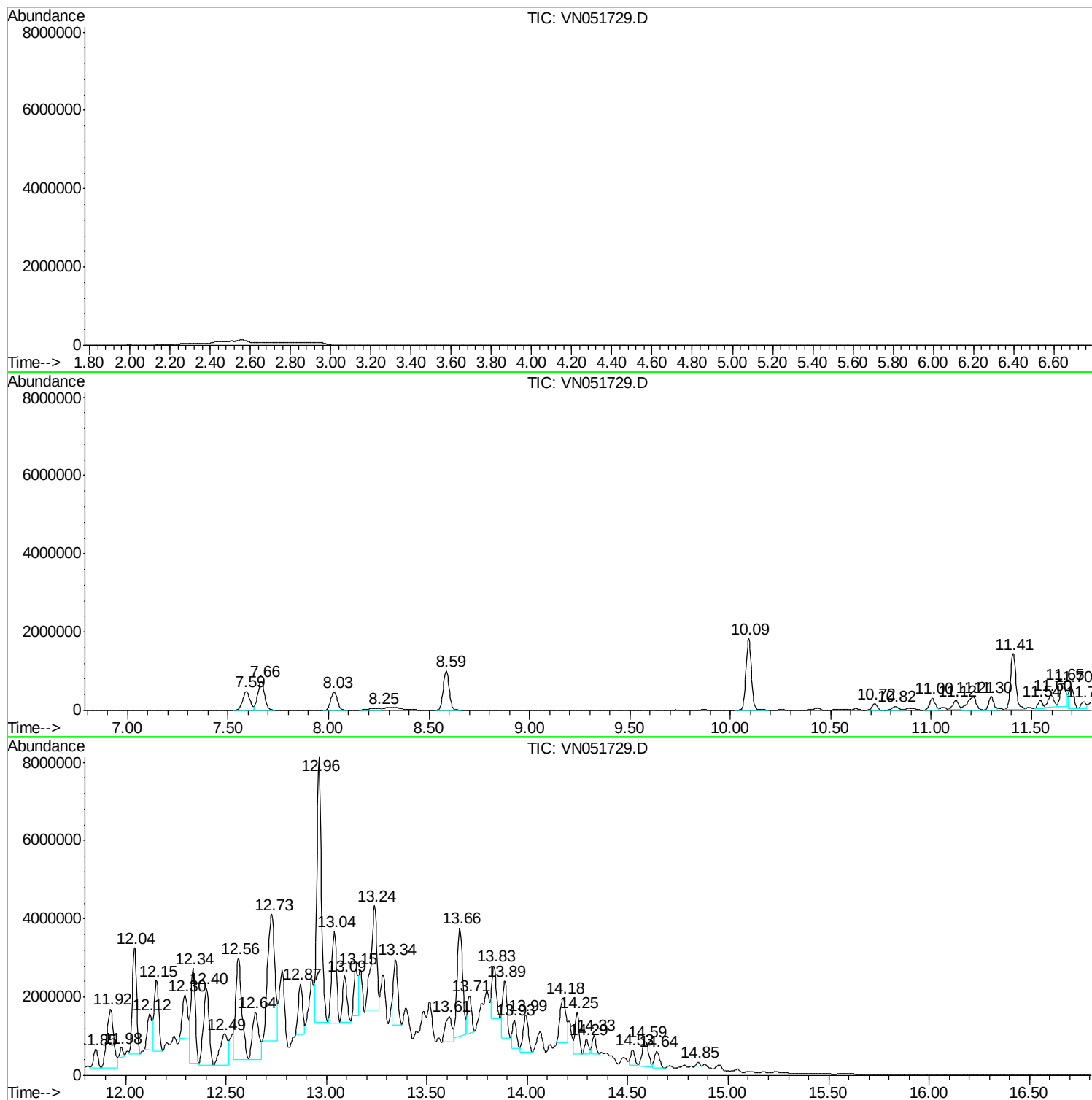
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ClientSampleId :
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N100418W.M
Quant Title : SW846 8260

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



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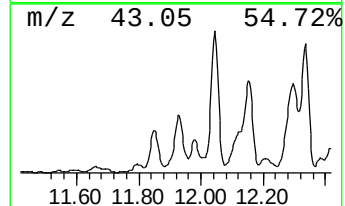
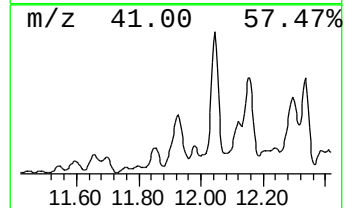
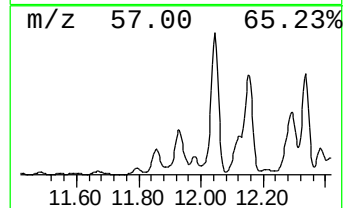
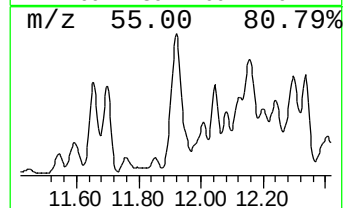
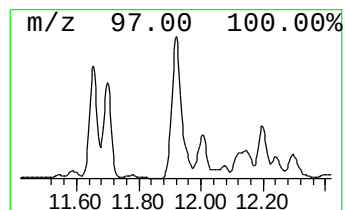
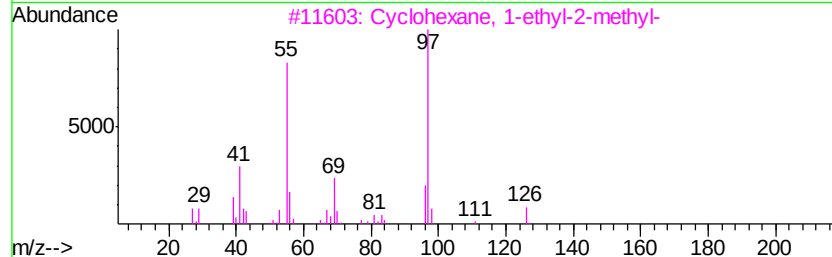
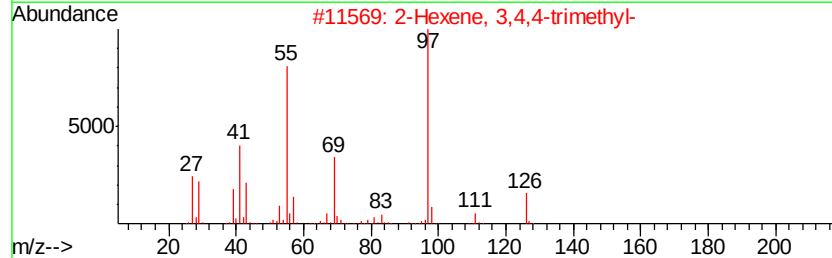
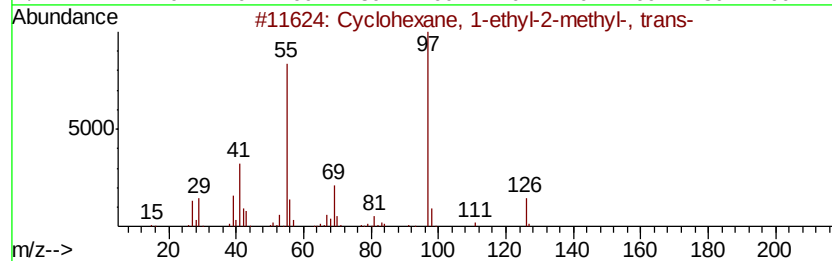
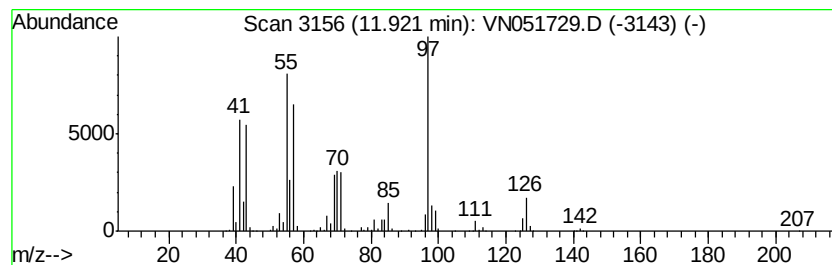
Instrument :
MSVOA_N
ClientSampleId :
EP1-MW-092718-FD-S

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-ethyl-2-meth... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.		
11.92	67.51 ug/l	3551880	Chlorobenzene-d5	11.41		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-78-8	55
2		2-Hexene, 3,4,4-trimethyl-	126	C9H18	053941-19-8	49
3		Cyclohexane, 1-ethyl-2-methyl-	126	C9H18	003728-54-9	49
4		4-Octen-3-one	126	C8H14O	014129-48-7	43
5		Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	006236-88-0	43



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ALS Vial : 12 Sample Multiplier: 28

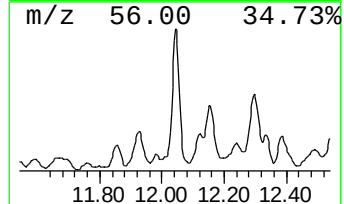
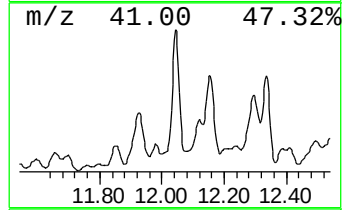
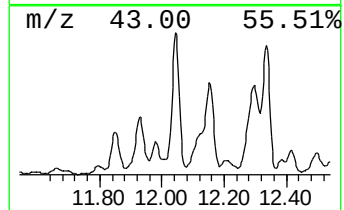
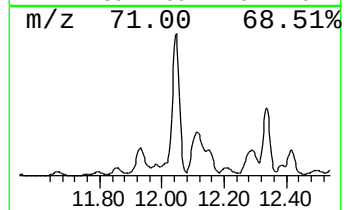
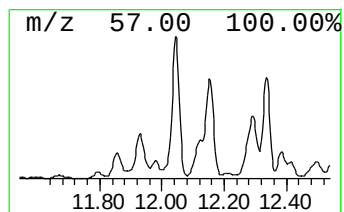
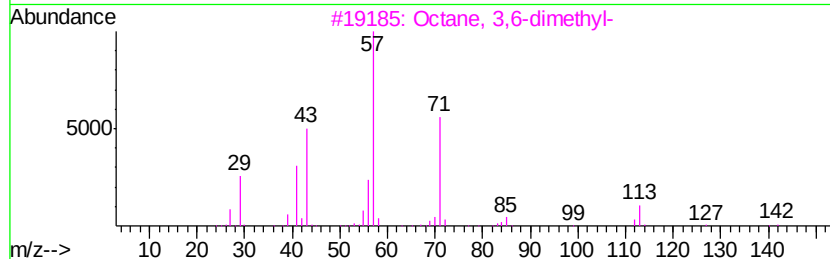
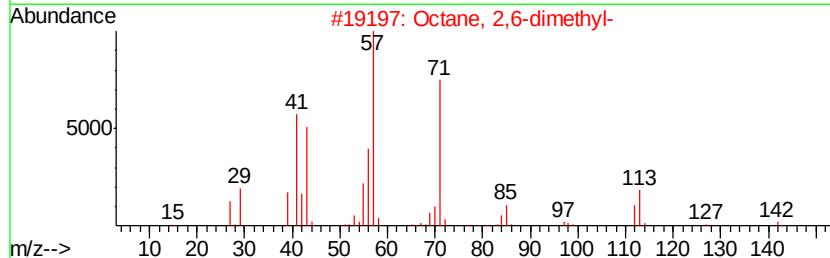
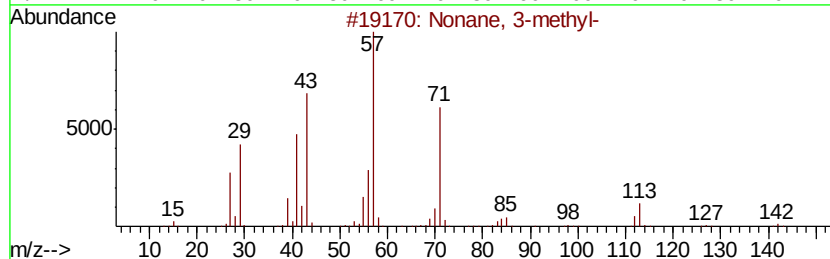
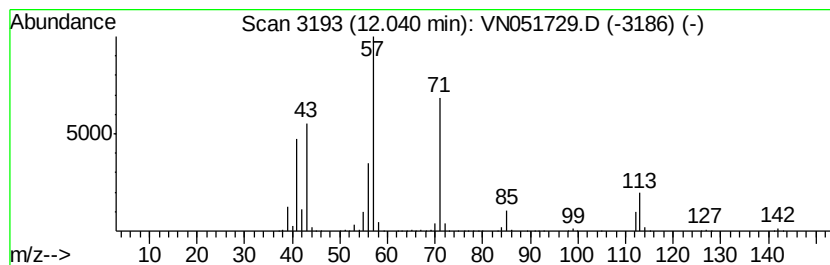
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N100418W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.		
12.04	72.70 ug/l	3824670	Chlorobenzene-d5	11.41		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Nonane, 3-methyl-	142	C10H22	005911-04-6	91
2		Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	90
3		Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	72
4		Octane, 1,1'-oxybis-	242	C16H34O	000629-82-3	64
5		Undecane, 6,6-dimethyl-	184	C13H28	017312-76-4	64



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Misc : 6.24g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 12 Sample Multiplier: 28

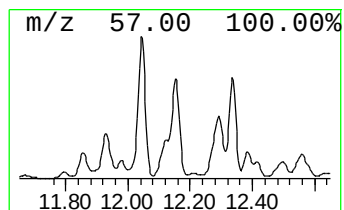
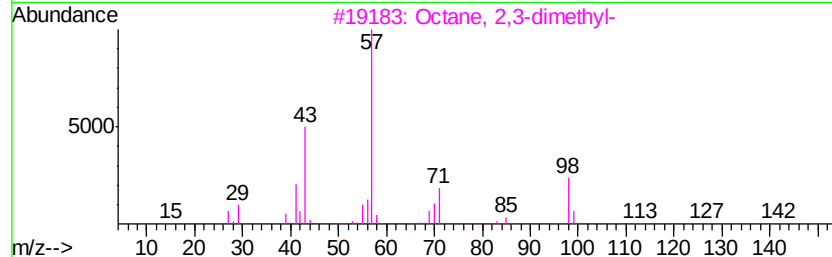
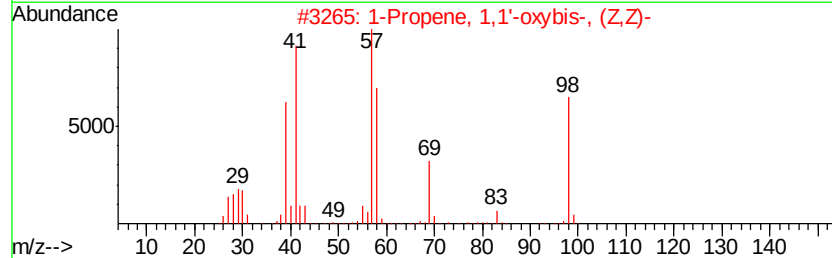
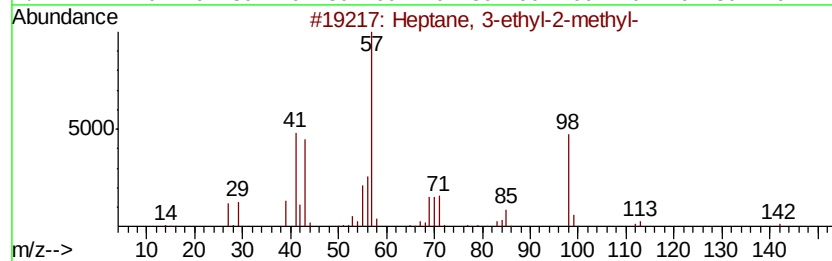
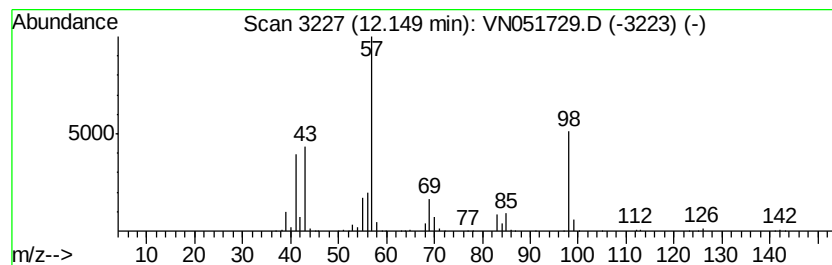
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 Heptane, 3-ethyl-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.15	54.68 ug/l	2876830	Chlorobenzene-d5	11.41
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Heptane, 3-ethyl-2-methyl-	142 C10H22	014676-29-0	80
2	1-Propene, 1,1'-oxybis-, (Z,Z)-	98 C6H100	004696-27-9	50
3	Octane, 2,3-dimethyl-	142 C10H22	007146-60-3	50
4	1-Propene, 1,1'-oxybis-, (E,Z)-	98 C6H100	004696-29-1	50
5	Ether, tert-butyl isopropylidene...	154 C10H180	024524-56-9	42



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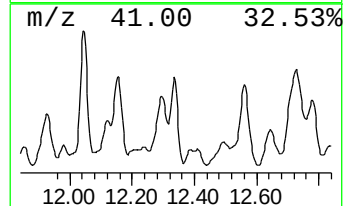
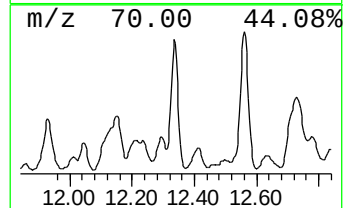
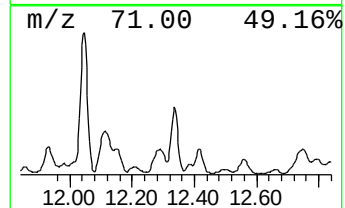
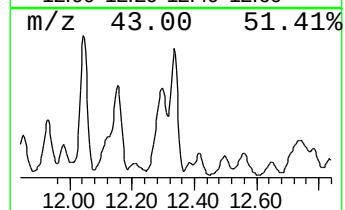
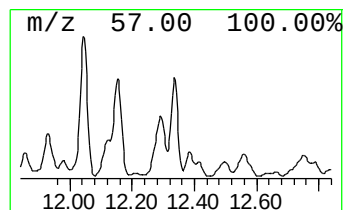
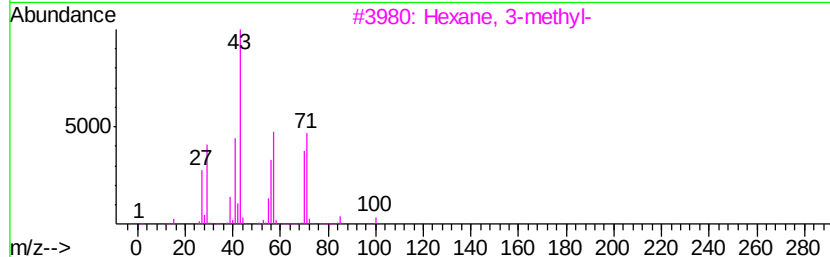
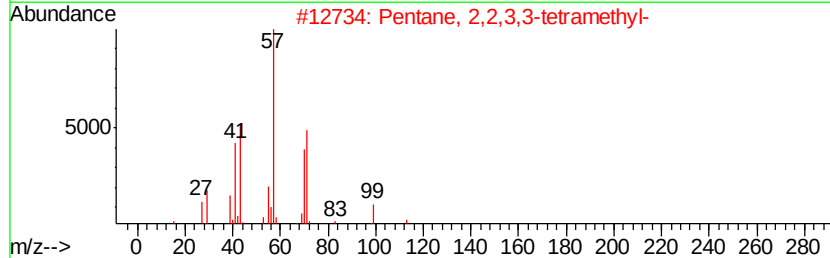
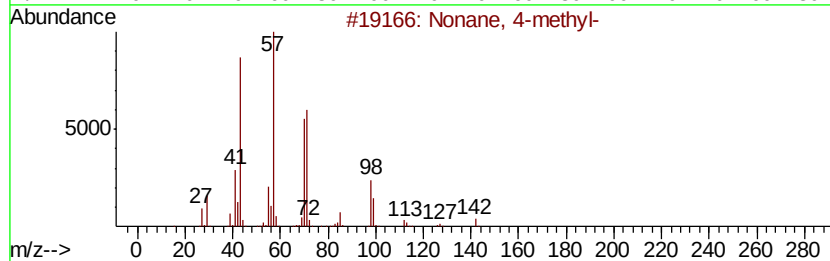
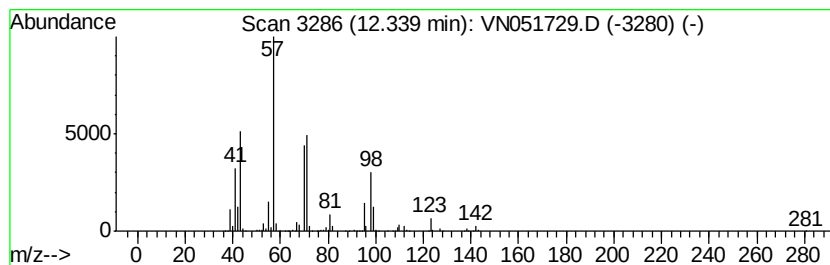
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Nonane, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.34	67.27 ug/l	3539310	Chlorobenzene-d5	11.41
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Nonane, 4-methyl-	142 C10H22	017301-94-9	64
2	Pentane, 2,2,3,3-tetramethyl-	128 C9H20	007154-79-2	53
3	Hexane, 3-methyl-	100 C7H16	000589-34-4	47
4	Octane, 3,5-dimethyl-	142 C10H22	015869-93-9	47
5	Pentane, 2,3,4-trimethyl-	114 C8H18	000565-75-3	38



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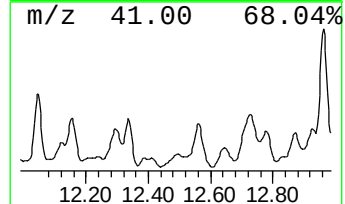
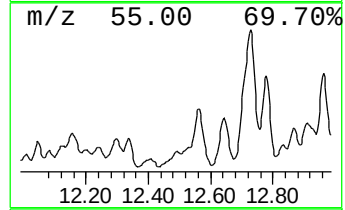
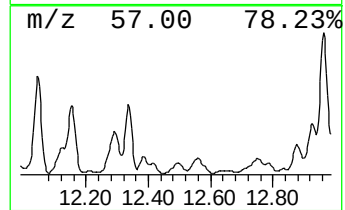
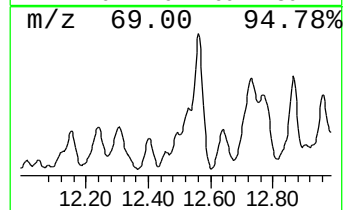
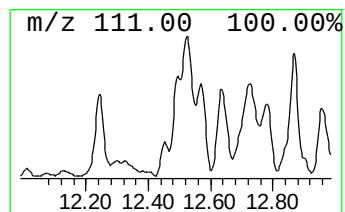
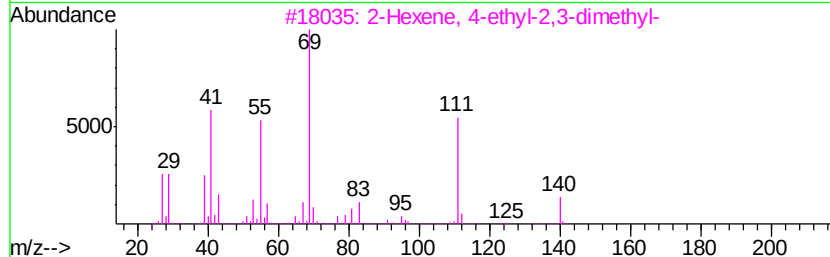
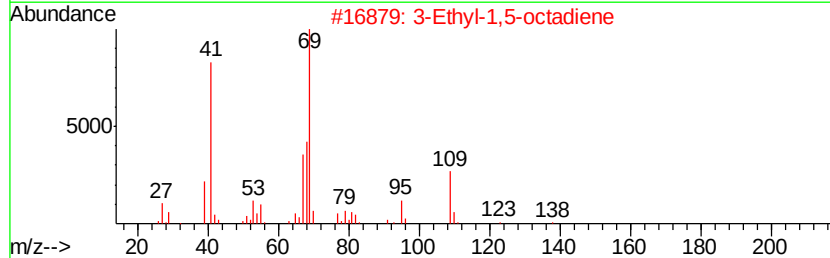
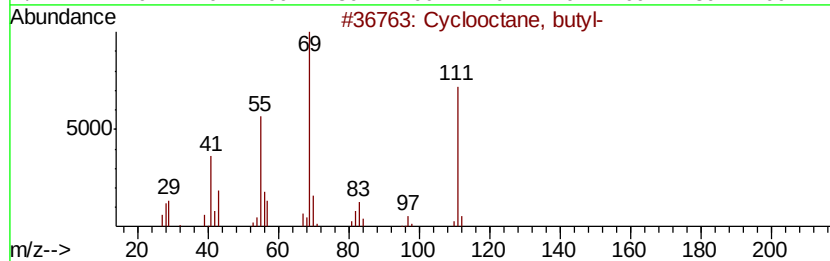
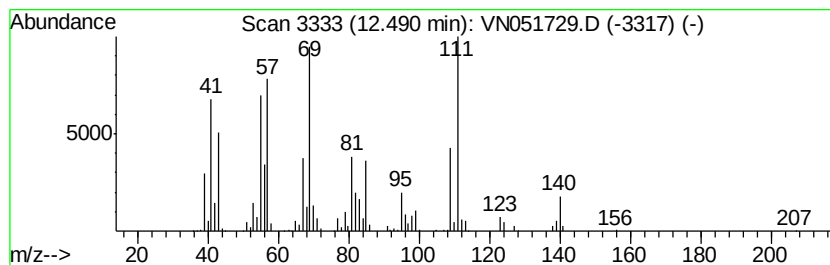
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Quant Title : SW846 8260

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

Peak Number 5 unknown12.49 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.49	43.03 ug/l	2206120	1,4-Dichlorobenzene-d4	13.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclooctane, butyl-	168	C12H24	016538-93-5	43
2		3-Ethyl-1,5-octadiene	138	C10H18	1000114-87-7	41
3		2-Hexene, 4-ethyl-2,3-dimethyl-	140	C10H20	1000149-19-7	38
4		3-Nonene, 3-methyl-, (E)-	140	C10H20	069405-42-1	27
5		3-Hexene, 2,5-dimethyl-, (E)-	112	C8H16	000692-70-6	22



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN100818\
Data File : VN051729.D
Acq On : 8 Oct 2018 12:31
Operator : MD\SY
Sample : J5165-02
Misc : 6.24g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 12 Sample Multiplier: 28

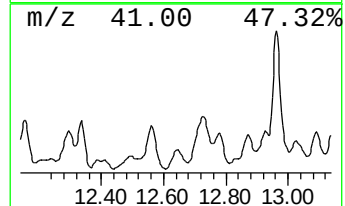
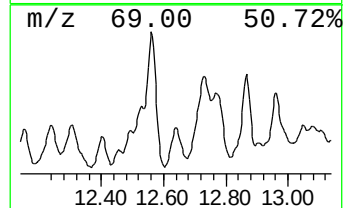
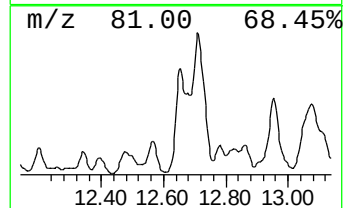
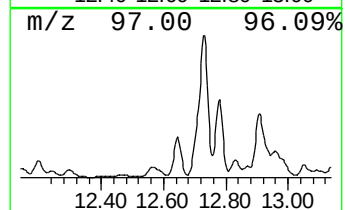
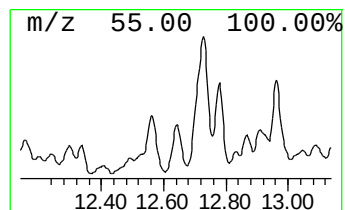
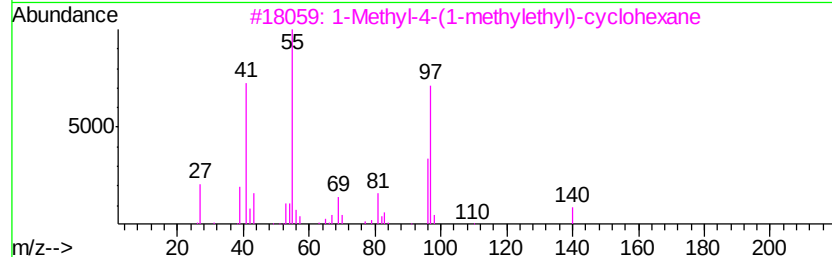
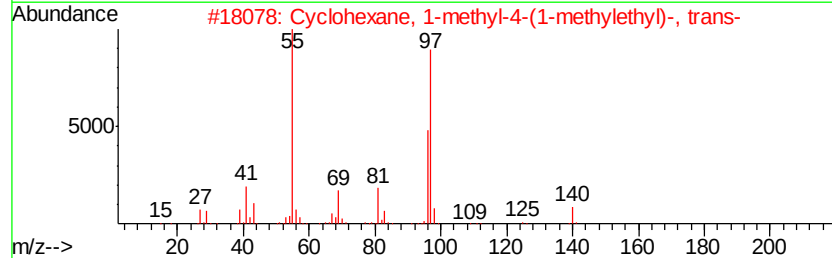
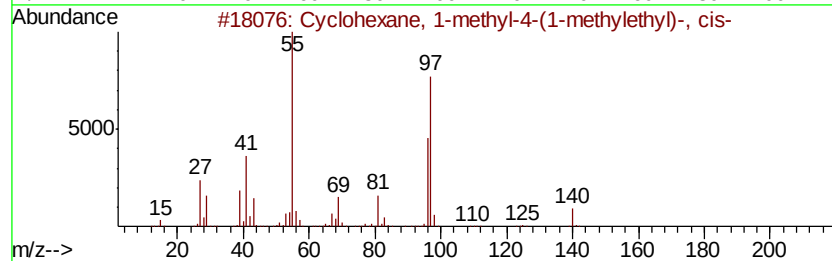
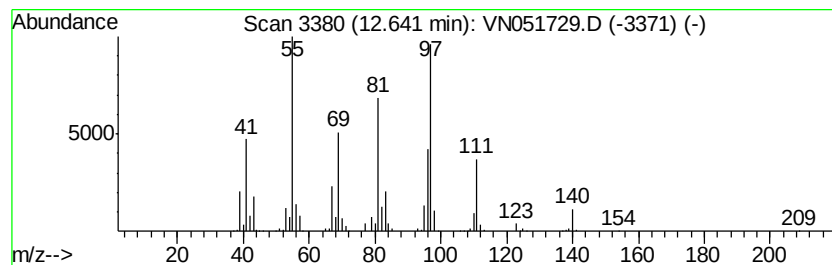
Instrument :
MSVOA_N
ClientSampleId :
EP1-MW-092718-FD-S

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-methyl-4-(1-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.64	52.47 ug/l	2690150	1,4-Dichlorobenzene-d4	13.35
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Cyclohexane, 1-methyl-4-(1-methy...	140 C10H20	006069-98-3 53
2		Cyclohexane, 1-methyl-4-(1-methy...	140 C10H20	001678-82-6 49
3		1-Methyl-4-(1-methylethyl)-cyclo...	140 C10H20	000099-82-1 46
4		Cyclohexane, 1-ethyl-4-methyl-, ...	126 C9H18	006236-88-0 43
5		Cyclohexane, 1-methyl-3-(1-methy...	140 C10H20	016580-24-8 43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN100818\
Data File : VN051729.D
Acq On : 8 Oct 2018 12:31
Operator : MD\SY
Sample : J5165-02
Misc : 6.24g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 12 Sample Multiplier: 28

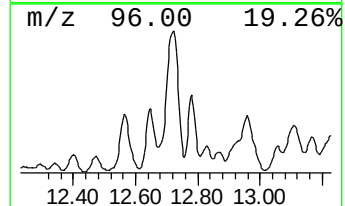
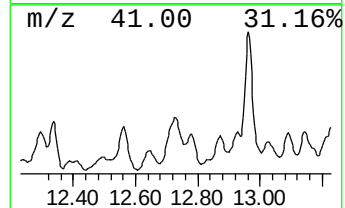
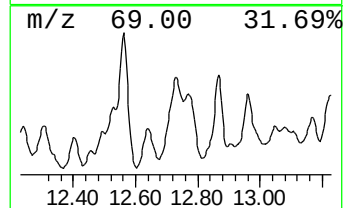
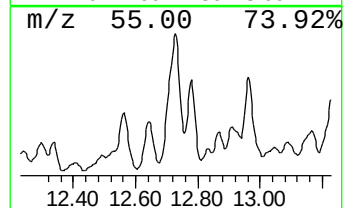
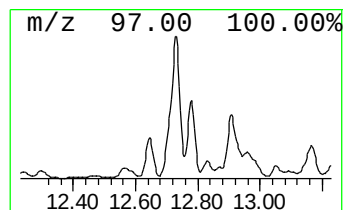
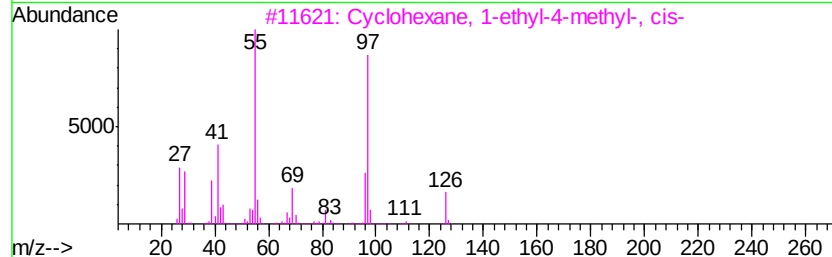
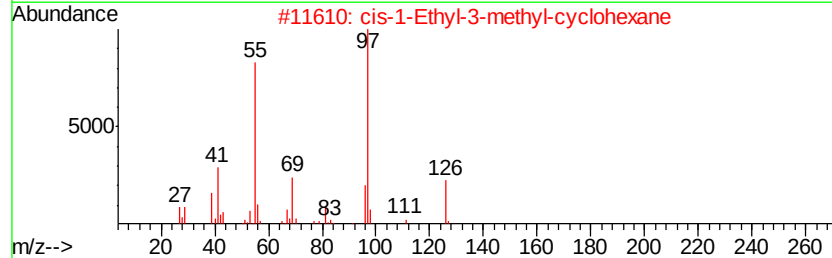
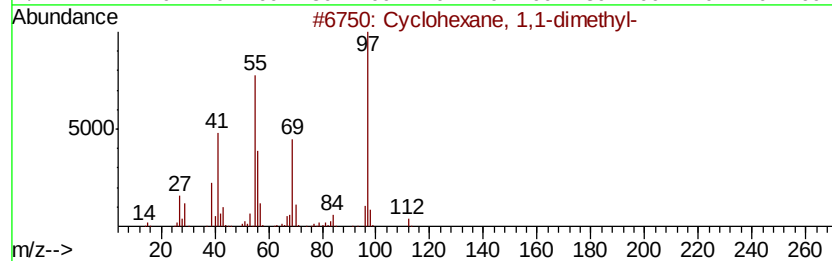
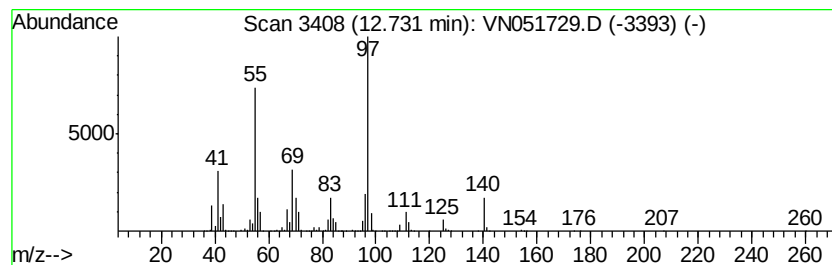
Instrument :
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ClientSampleId :
EP1-MW-092718-FD-S

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 Cyclohexane, 1,1-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.73	158.44 ug/l	8123210	1,4-Dichlorobenzene-d4	13.35
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Cyclohexane, 1,1-dimethyl-	112 C8H16	000590-66-9 70
2		cis-1-Ethyl-3-methyl-cyclohexane	126 C9H18	019489-10-2 59
3		Cyclohexane, 1-ethyl-4-methyl-, ...	126 C9H18	004926-78-7 59
4		Cyclohexane, 1-ethyl-2-methyl-	126 C9H18	003728-54-9 59
5		1-Ethyl-3-methylcyclohexane (c,t)	126 C9H18	003728-55-0 59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN100818\
Data File : VN051729.D
Acq On : 8 Oct 2018 12:31
Operator : MD\SY
Sample : J5165-02
Misc : 6.24g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 12 Sample Multiplier: 28

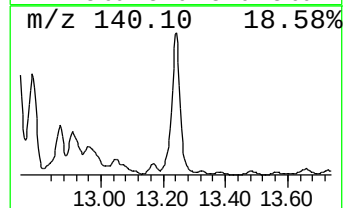
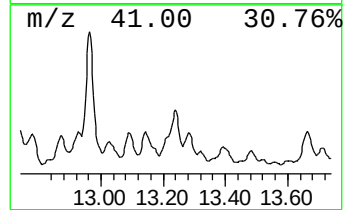
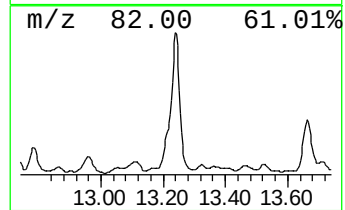
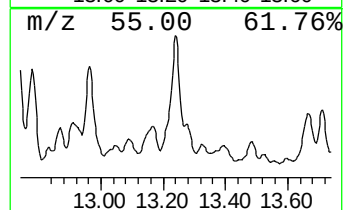
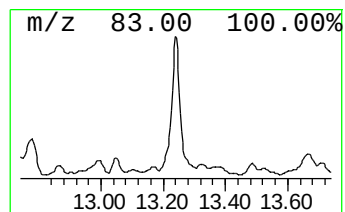
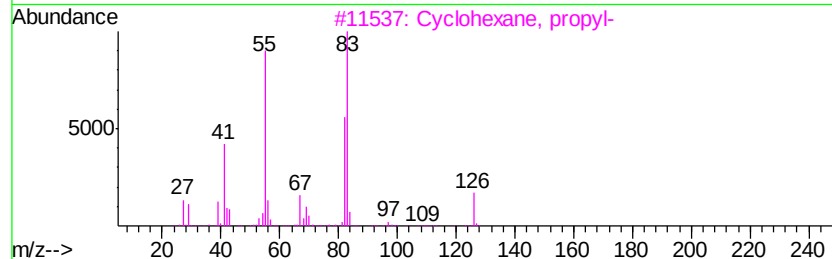
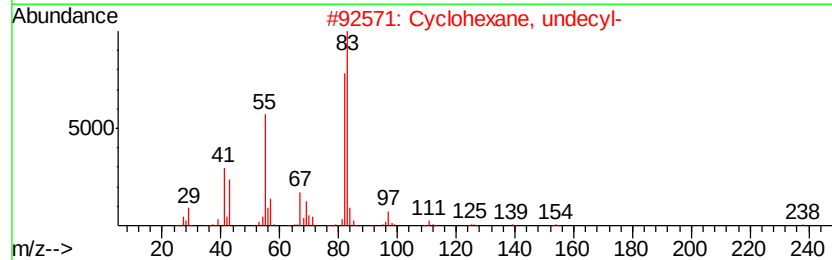
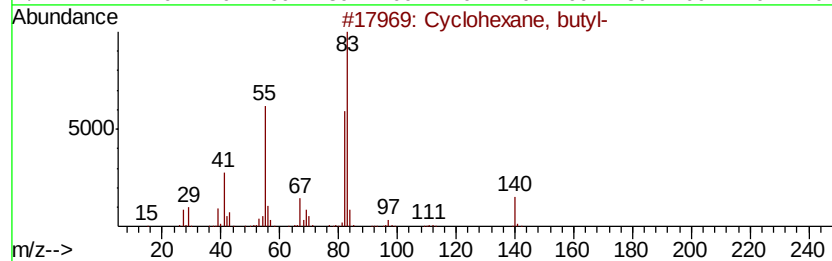
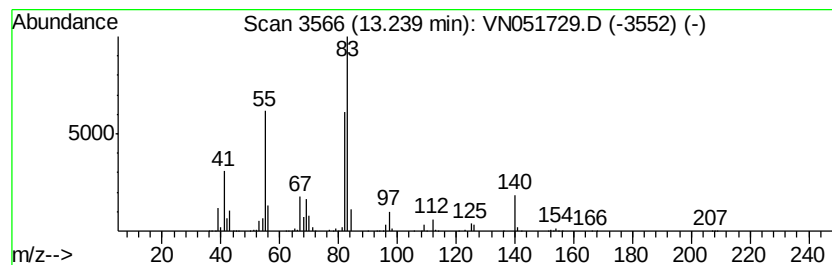
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EP1-MW-092718-FD-S

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 8 Cyclohexane, butyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.24	101.89 ug/l	5223850	1,4-Dichlorobenzene-d4	13.35
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Cyclohexane, butyl-	140 C10H20	001678-93-9 93
2		Cyclohexane, undecyl-	238 C17H34	054105-66-7 86
3		Cyclohexane, propyl-	126 C9H18	001678-92-8 83
4		Cyclohexane, ethyl-	112 C8H16	001678-91-7 80
5		Cyclohexane, pentyl-	154 C11H22	004292-92-6 80



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN100818\
Data File : VN051729.D
Acq On : 8 Oct 2018 12:31
Operator : MD\SY
Sample : J5165-02
Misc : 6.24g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 12 Sample Multiplier: 28

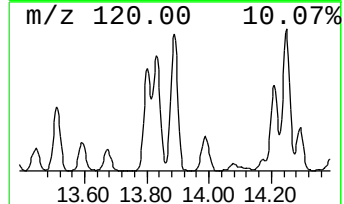
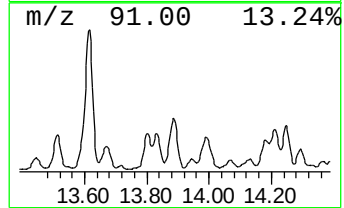
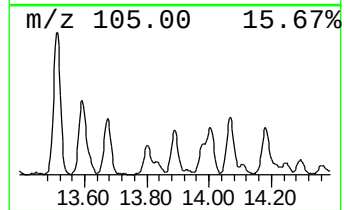
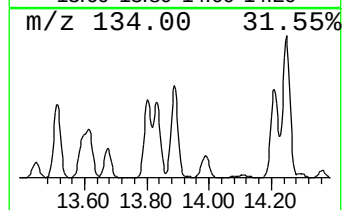
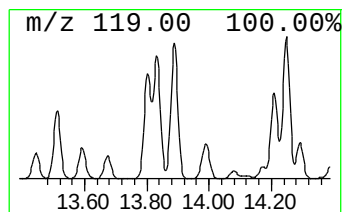
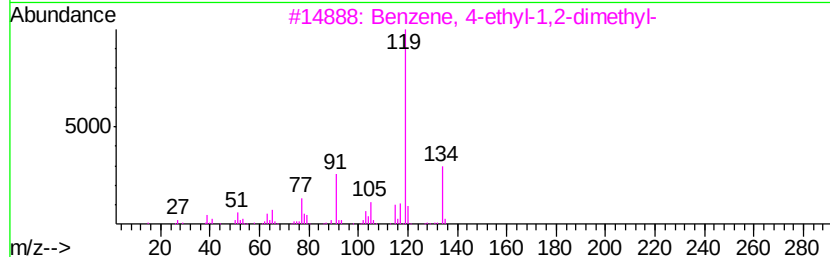
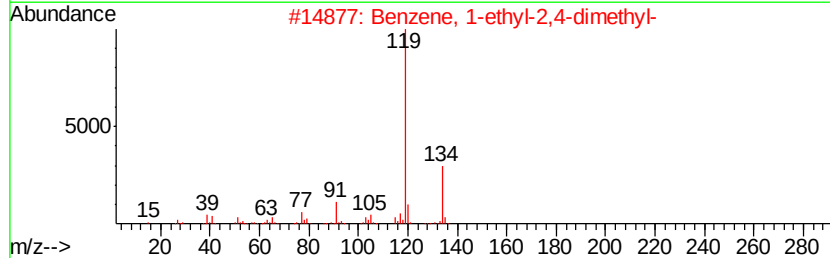
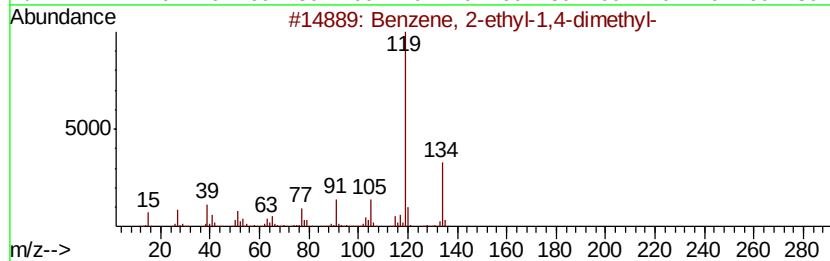
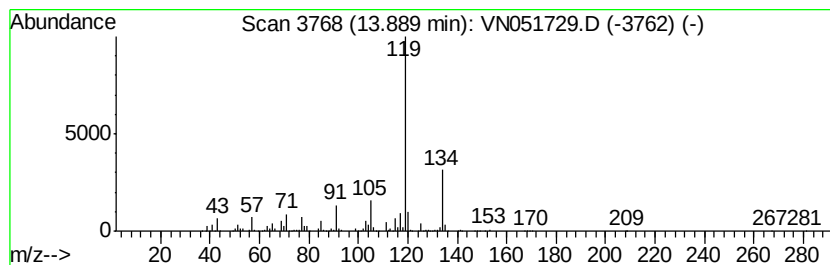
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EP1-MW-092718-FD-S

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 9 Benzene, 2-ethyl-1,4-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.89	43.72 ug/l	2241520	1,4-Dichlorobenzene-d4	13.35	
Hit# of	5	Tentative ID	MW MolForm	CAS#	Qual
1	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	94
2	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	94
3	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	93
4	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	93
5	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	93



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN100818\
Data File : VN051729.D
Acq On : 8 Oct 2018 12:31
Operator : MD\SY
Sample : J5165-02
Misc : 6.24g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 12 Sample Multiplier: 28

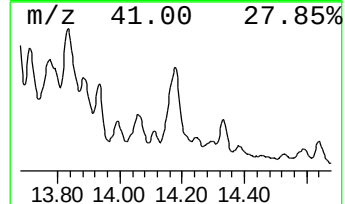
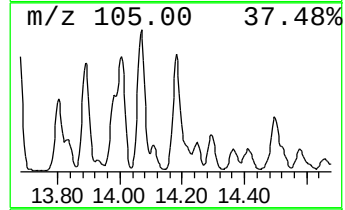
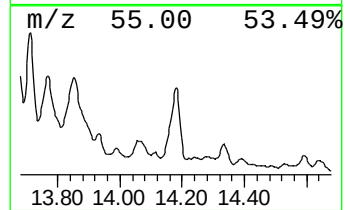
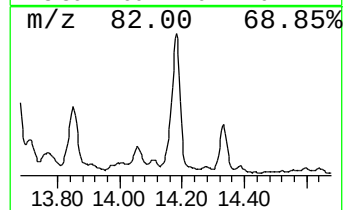
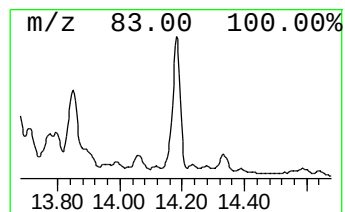
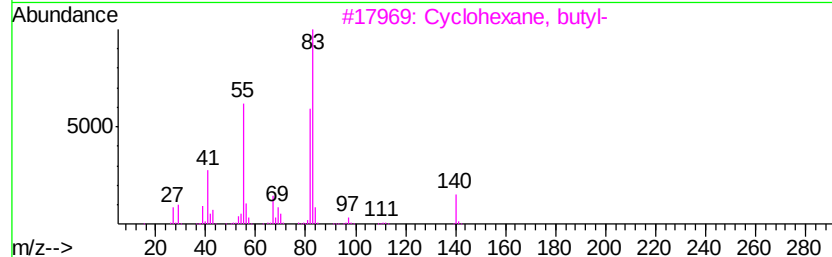
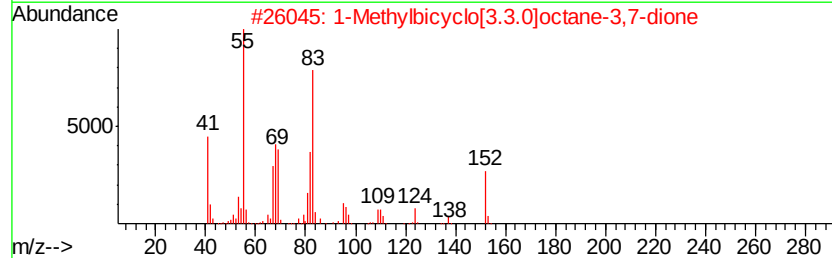
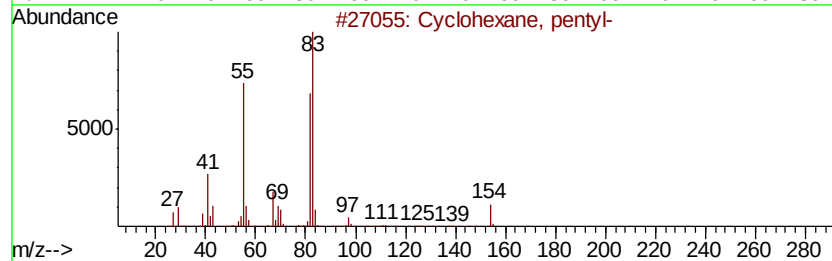
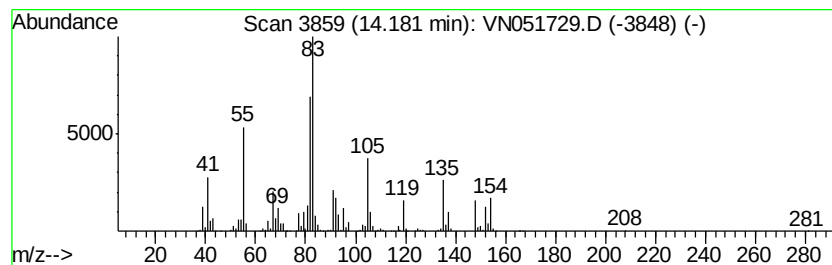
Instrument :
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ClientSampleId :
EP1-MW-092718-FD-S

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 10 Cyclohexane, pentyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.18	45.94 ug/l	2355490	1,4-Dichlorobenzene-d4	13.35
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Cyclohexane, pentyl-	154 C11H22	004292-92-6 60
2		1-Methylbicyclo[3.3.0]octane-3,7...	152 C9H12O2	021170-08-1 53
3		Cyclohexane, butyl-	140 C10H20	001678-93-9 43
4		Cyclohexane, 2-propenyl-	124 C9H16	002114-42-3 43
5		Cyclohexane, octyl-	196 C14H28	001795-15-9 43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN100818\
Data File : VN051729.D
Acq On : 8 Oct 2018 12:31
Operator : MD\SY
Sample : J5165-02
Misc : 6.24g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 12 Sample Multiplier: 28

Instrument :
MSVOA_N
ClientSampleId :
EP1-MW-092718-FD-S

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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Nonane, 3-methyl-	12.04	72.7	ug/l	3824670	3	11.41	2630600	50.0
Heptane, 3-ethyl-...	12.15	54.7	ug/l	2876830	3	11.41	2630600	50.0
Nonane, 4-methyl-	12.34	67.3	ug/l	3539310	3	11.41	2630600	50.0
unknown12.49	12.49	43.0	ug/l	2206120	4	13.35	2563440	50.0
Cyclohexane, 1-me...	12.64	52.5	ug/l	2690150	4	13.35	2563440	50.0
Cyclohexane, 1,1-...	12.73	158.4	ug/l	8123210	4	13.35	2563440	50.0
Cyclohexane, butyl-	13.24	101.9	ug/l	5223850	4	13.35	2563440	50.0
Benzene, 2-ethyl-...	13.89	43.7	ug/l	2241520	4	13.35	2563440	50.0
Cyclohexane, pentyl-	14.18	45.9	ug/l	2355490	4	13.35	2563440	50.0