LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN090718\
Data File : VN051057.D
Acq On : 7 Sep 2018 16:40
Operator : MD\SY
Sample : J4693-15 5X
Misc : 5.51g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : EP1-MW-D(10-15)

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\82N082118W.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	1790	1809	1821	rBV	475157	1202587	2.44%	0.249%
2	7.667	1821	1833	1872	rVB2	752646	1782987	3.62%	0.370%
3	8.027	1925	1945	1972	rBV	468144	1093015	2.22%	0.227%
4	8.587	2103	2119	2147	rBV	1061223	2192853	4.45%	0.455%
5	10.091	2572	2587	2614	rBV3	2520960	5205400	10.57%	1.080%
6	10.432	2684	2693	2709	rVB	529736	999353	2.03%	0.207%
7	10.532	2709	2724	2732	rBV2	279370	601451	1.22%	0.125%
8	10.628	2746	2754	2763	rVB	311481	494424	1.00%	0.103%
9	10.718	2764	2782	2794	rVB	953776	1642500	3.34%	0.341%
10	10.821	2800	2814	2827	rBV	814633	1696154	3.44%	0.352%
11	10.889	2827	2835	2842	rBV2	375441	661034	1.34%	0.137%
12	10.953	2847	2855	2862	rVV	1039467	1756284	3.57%	0.364%
13	11.005	2862	2871	2882	rVV	2474999	4516642	9.17%	0.937%
14	11.059	2882	2888	2896	rVV	496167	758515	1.54%	0.157%
15	11.124	2896	2908	2916	rVV3	1897030	3516334	7.14%	0.730%
16	11.165	2917	2921	2927	rVV2	654721	952889	1.94%	0.198%
17	11.214	2927	2936	2951	rVB	2328143	4284458	8.70%	0.889%
18	11.291	2951	2960	2968	rBV	659373	1113988	2.26%	0.231%
19	11.406	2984	2996	3006	rBV2	1688650	3342647	6.79%	0.693%
20	11.493	3014	3023	3030	rBV4	529094	1040746	2.11%	0.216%
21	11.542	3031	3038	3045	rBV	1326081	1922239	3.90%	0.399%
22	11.596	3045	3055	3063	rBV7	1942887	4113464	8.35%	0.853%
23	11.657	3064	3074	3081	rVV2	7064138	12506274	25.40%	2.595%
24	11.699	3082	3087	3097	rVB3	5062663	7869883	15.98%	1.633%
25	11.760	3097	3106	3111	rBV3	1121667	1956658	3.97%	0.406%
26	11.812	3113	3122	3127	rBV3	833158	1601237	3.25%	0.332%
27	11.853	3127	3135	3143	rVB3	3721984	5660728	11.50%	1.174%
28	11.924	3143	3157	3169	rBV6	11703785	28287715	57.45%	5.869%
29	12.046	3187	3195	3203	rBV	14612049	19672727	39.96%	4.081%
30	12.120	3210	3218	3224	rBV4	8961610	15313272	31.10%	3.177%
31	12.165	3224	3232	3250	rVB4	16245943	32793145	66.60%	6.803%
32	12.403	3296	3306	3316	rBV7	3980700	7851175	15.95%	1.629%
33	12.490	3317	3333	3340	rBV7	4634511	13516711	27.45%	2.804%
34	12.564	3349	3356	3371	rVB4	12907889	27611458	56.08%	5.728%

LSC Area Percent Report

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Operator : MD\SY
Sample : J4693-15 5X
Misc : 5.51g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : EP1-MW-D(10-15)

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\82N082118W.M
Title : SW846 8260

35	12.651	3371	3383	3389	rBV8	7299003	15303525	31.08%	3.175%
36	12.731	3404	3408	3417	rVB2	19283650	27149762	55.14%	5.633%
37	12.783	3418	3424	3434	rVB3	9078643	14448258	29.34%	2.997%
38	12.869	3445	3451	3458	rBV5	4537979	6104834	12.40%	1.267%
39	12.963	3473	3480	3493	rVB3	18827674	31339274	63.65%	6.502%
40	13.040	3494	3504	3514	rBV2	29666506	49237106	100.00%	10.215%
41	13.168	3533	3544	3552	rVB6	4769311	11053524	22.45%	2.293%
42	13.242	3553	3567	3574	rBV2	12101924	22599803	45.90%	4.689%
43	13.374	3603	3608	3624	rVB	4301618	7423210	15.08%	1.540%
44	13.596	3669	3677	3688	rBV2	3803868	8424548	17.11%	1.748%
45	13.664	3689	3698	3708	rVV5	10294124	17889032	36.33%	3.711%
46	13.712	3709	3713	3721	rVB2	2519868	3152557	6.40%	0.654%
47	13.773	3725	3732	3734	rBV5	1965634	2513810	5.11%	0.522%
48	13.834	3746	3751	3760	rVV5	4257996	6080071	12.35%	1.261%
49	13.889	3762	3768	3777	rVB	5903844	9129627	18.54%	1.894%
50	13.995	3792	3801	3810	rVB4	2930039	5049725	10.26%	1.048%
51	14.178	3848	3858	3874	rBV8	3778635	9901883	20.11%	2.054%
52	14.249	3875	3880	3888	rVB	2515612	3324615	6.75%	0.690%
53	14.294	3888	3894	3899	rBV3	1016001	1356946	2.76%	0.282%
54	14.332	3900	3906	3914	rVB	1817611	2380558	4.83%	0.494%
55	14.525	3961	3966	3974	rVB2	888358	1190467	2.42%	0.247%
56	14.583	3974	3984	3996	rVV2	2931028	5611780	11.40%	1.164%
57	14.644	3996	4003	4015	rVB3	1048073	1818461	3.69%	0.377%

Sum of corrected areas: 482014323

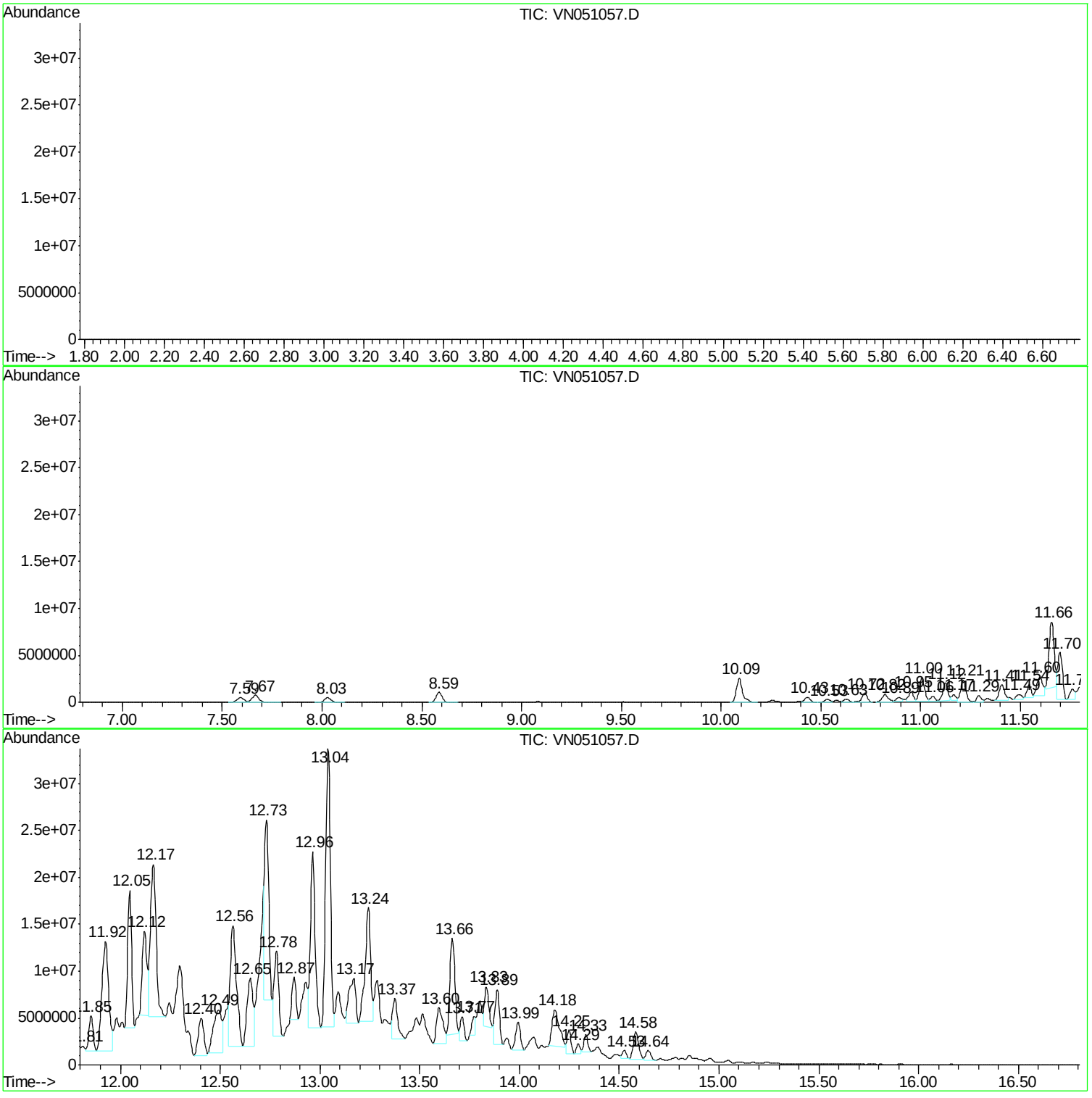
LSC Report - Integrated Chromatogram

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN090718\
Data File : VN051057.D
Acq On : 7 Sep 2018 16:40
Operator : MD\SY
Sample : J4693-15 5X
Misc : 5.51g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
EP1-MW-D(10-15)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N082118W.M
Quant Title : SW846 8260

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



Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN090718\
Data File : VN051057.D
Acq On : 7 Sep 2018 16:40
Operator : MD\SY
Sample : J4693-15 5X
Misc : 5.51g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : EP1-MW-D(10-15)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N082118W.M
Quant Title : SW846 8260

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

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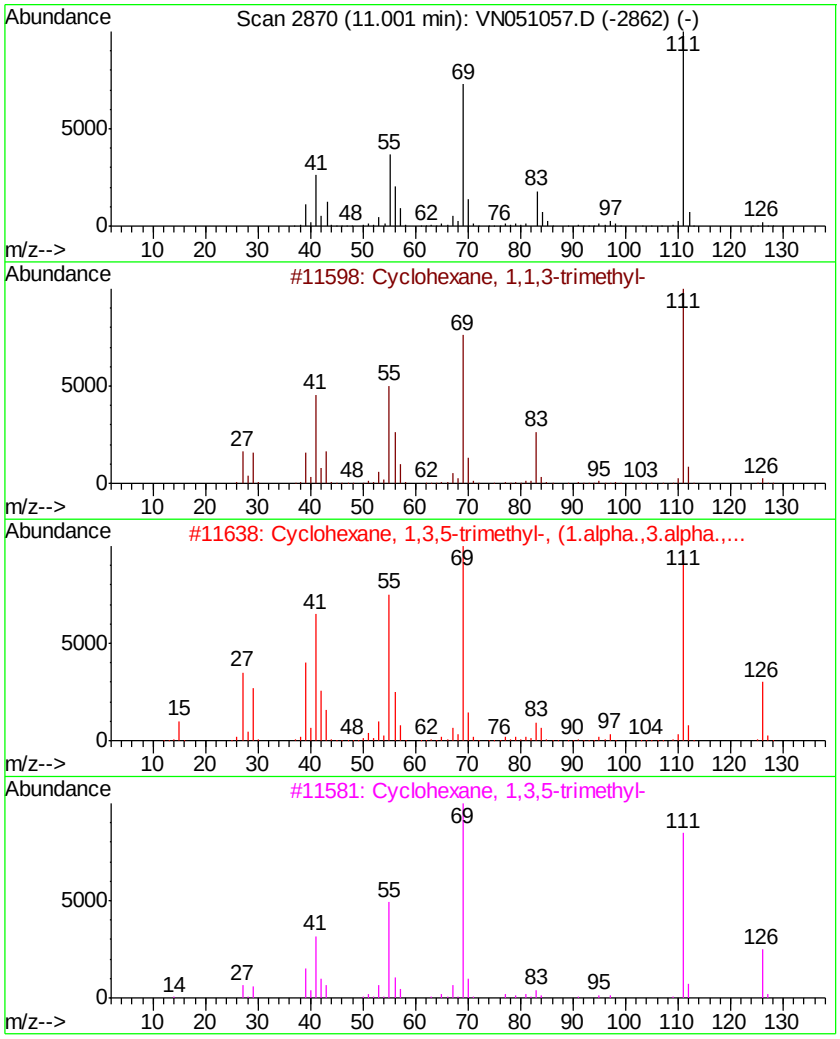
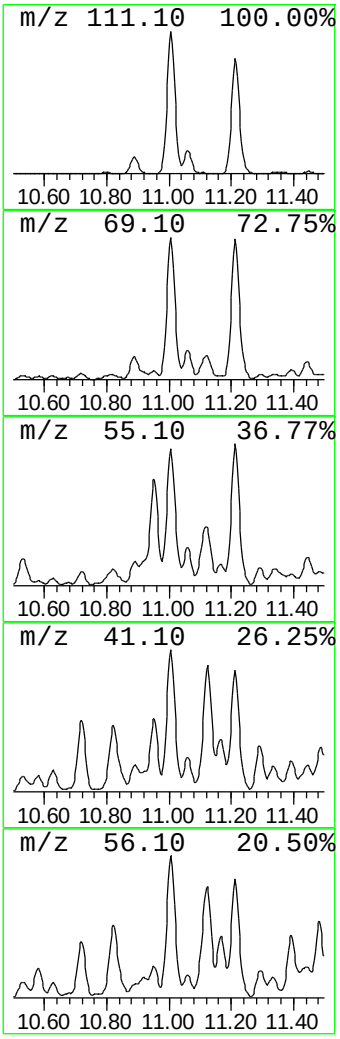
Peak Number 1 Cyclohexane, 1,1,3-trimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.00	67.56 ug/l	4516640	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	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	59
4	4-Amino-6-hydroxypyrimidine	111	C4H5N3O	001193-22-2	53
5	p-Fluoroaniline	111	C6H6FN	000371-40-4	50





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN090718\
Data File : VN051057.D
Acq On : 7 Sep 2018 16:40
Operator : MD\SY
Sample : J4693-15 5X
Misc : 5.51g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : EP1-MW-D(10-15)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N082118W.M
Quant Title : SW846 8260

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

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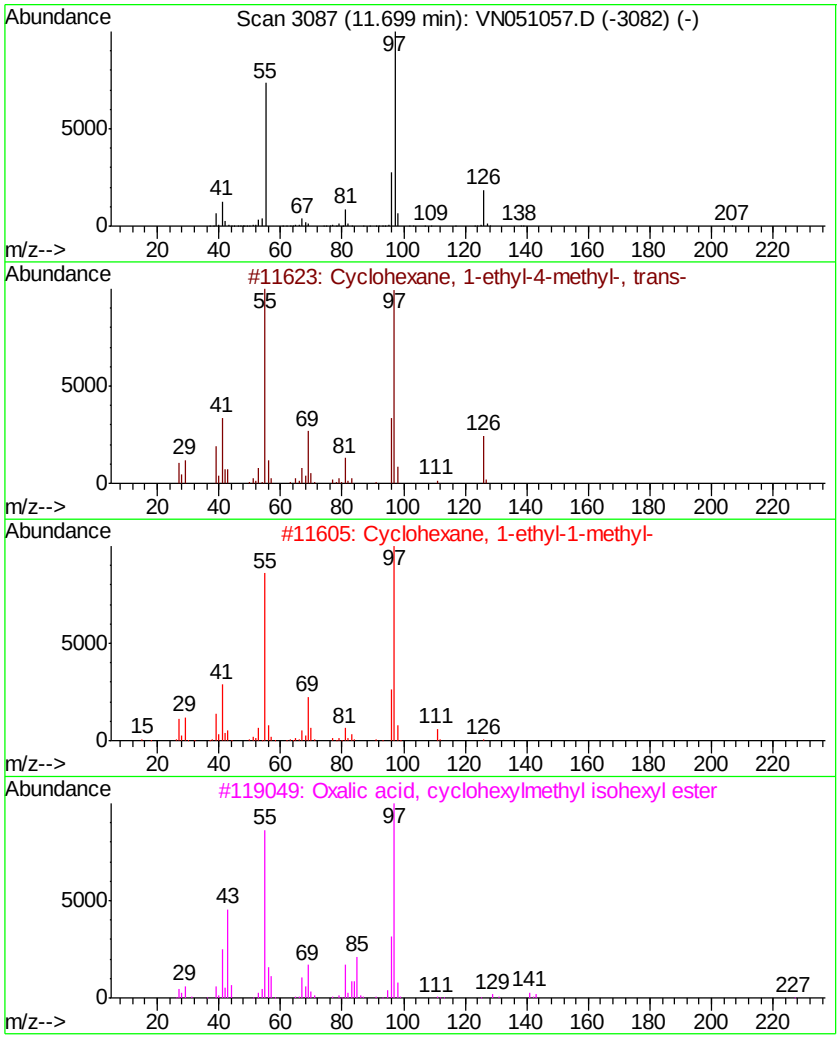
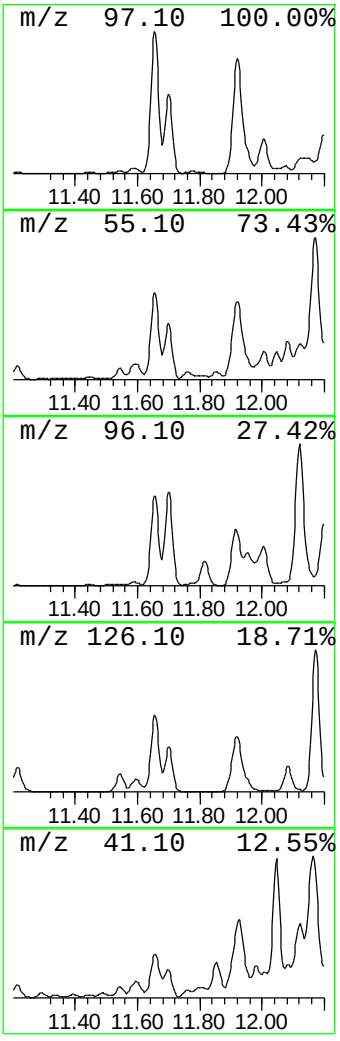
Peak Number 2 Cyclohexane, 1-ethyl-4-meth... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.70	117.72 ug/l	7869880	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	006236-88-0	86
2	Cyclohexane, 1-ethyl-1-methyl-	126	C9H18	004926-90-3	72
3	Oxalic acid, cyclohexylmethyl is...	270	C15H26O4	1000309-68-3	56
4	Cyclohexane, 1-bromo-4-methyl-	176	C7H13Br	006294-40-2	50
5	Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	004926-78-7	50





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN090718\
Data File : VN051057.D
Acq On : 7 Sep 2018 16:40
Operator : MD\SY
Sample : J4693-15 5X
Misc : 5.51g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : EP1-MW-D(10-15)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N082118W.M
Quant Title : SW846 8260

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

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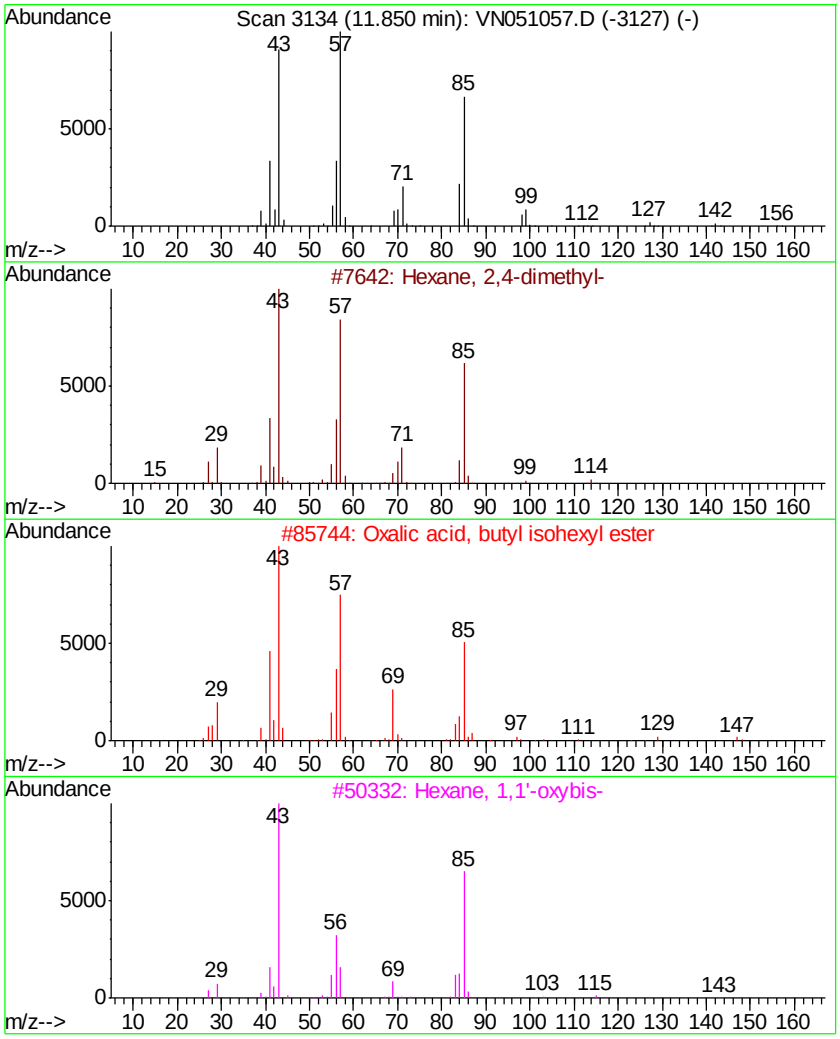
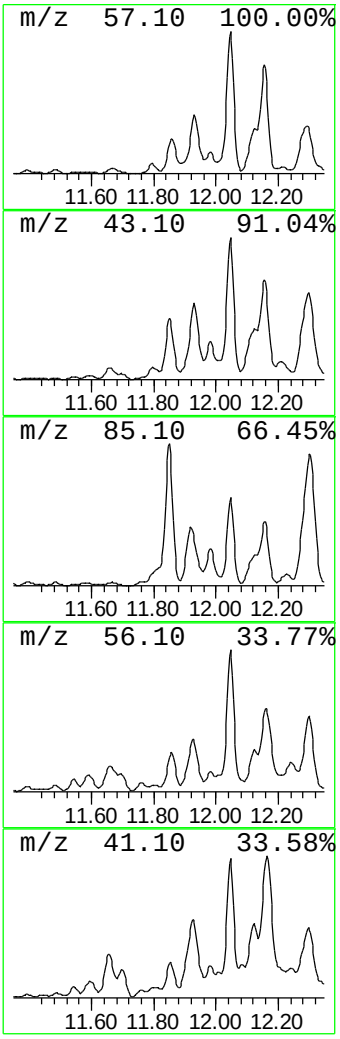
Peak Number 3 Hexane, 2,4-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.85	84.67 ug/l	5660730	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	Oxalic acid, butyl isohexyl ester	230	C12H22O4	1000309-32-7	59
3	Hexane, 1,1'-oxybis-	186	C12H26O	000112-58-3	53
4	Nonane, 2,5-dimethyl-	156	C11H24	017302-27-1	50
5	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	50





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN090718\
Data File : VN051057.D
Acq On : 7 Sep 2018 16:40
Operator : MD\SY
Sample : J4693-15 5X
Misc : 5.51g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : EP1-MW-D(10-15)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N082118W.M
Quant Title : SW846 8260

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

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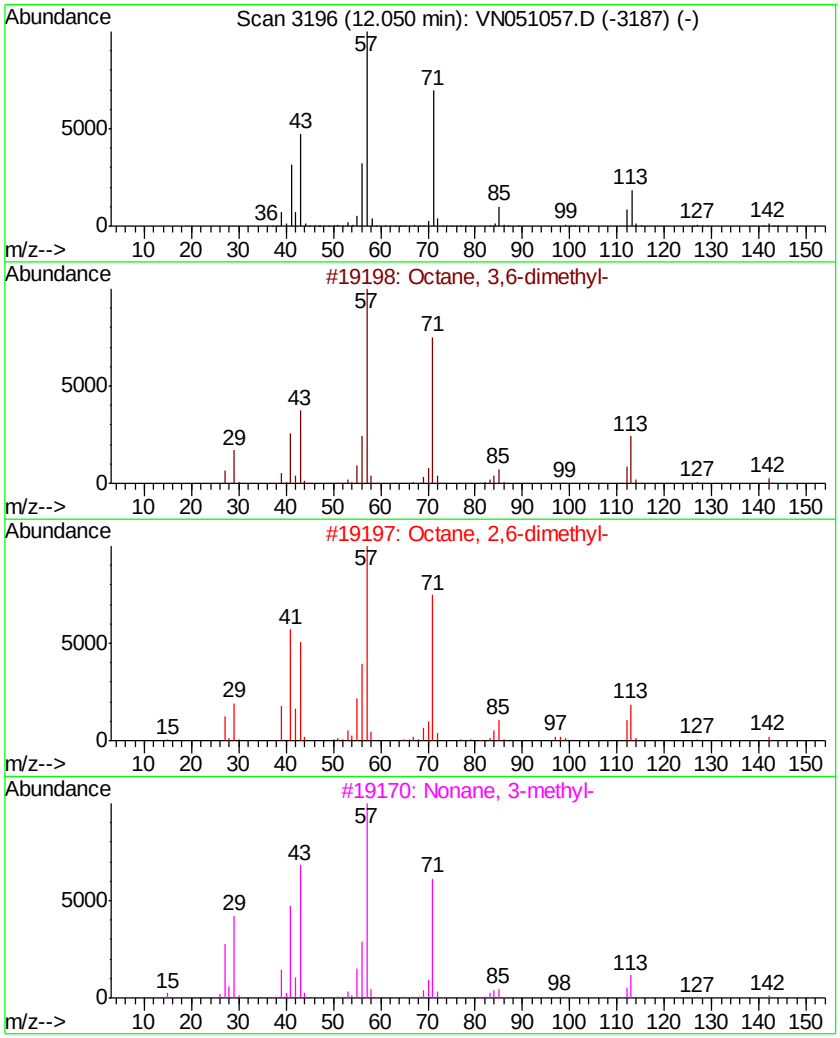
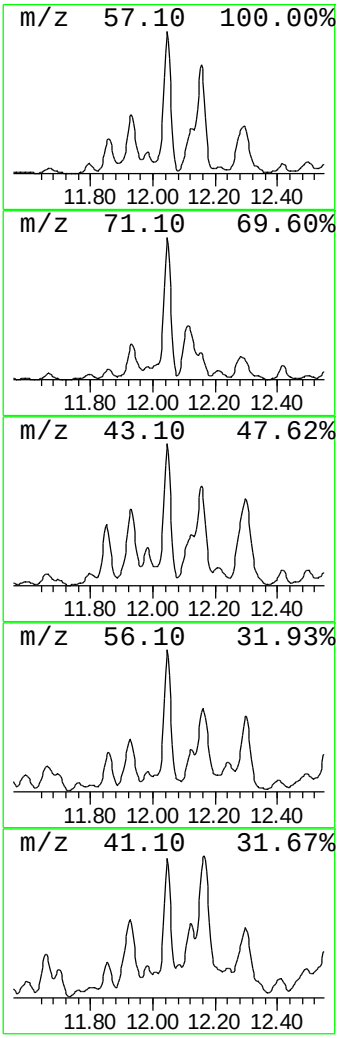
Peak Number 5 Octane, 3,6-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.05	294.27 ug/l	19672700	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	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	90
4	Undecane, 6,6-dimethyl-	184	C13H28	017312-76-4	64
5	Sulfurous acid, 2-ethylhexyl hex...	418	C24H50O3S	1000309-19-9	64





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN090718\
Data File : VN051057.D
Acq On : 7 Sep 2018 16:40
Operator : MD\SY
Sample : J4693-15 5X
Misc : 5.51g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : EP1-MW-D(10-15)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N082118W.M
Quant Title : SW846 8260

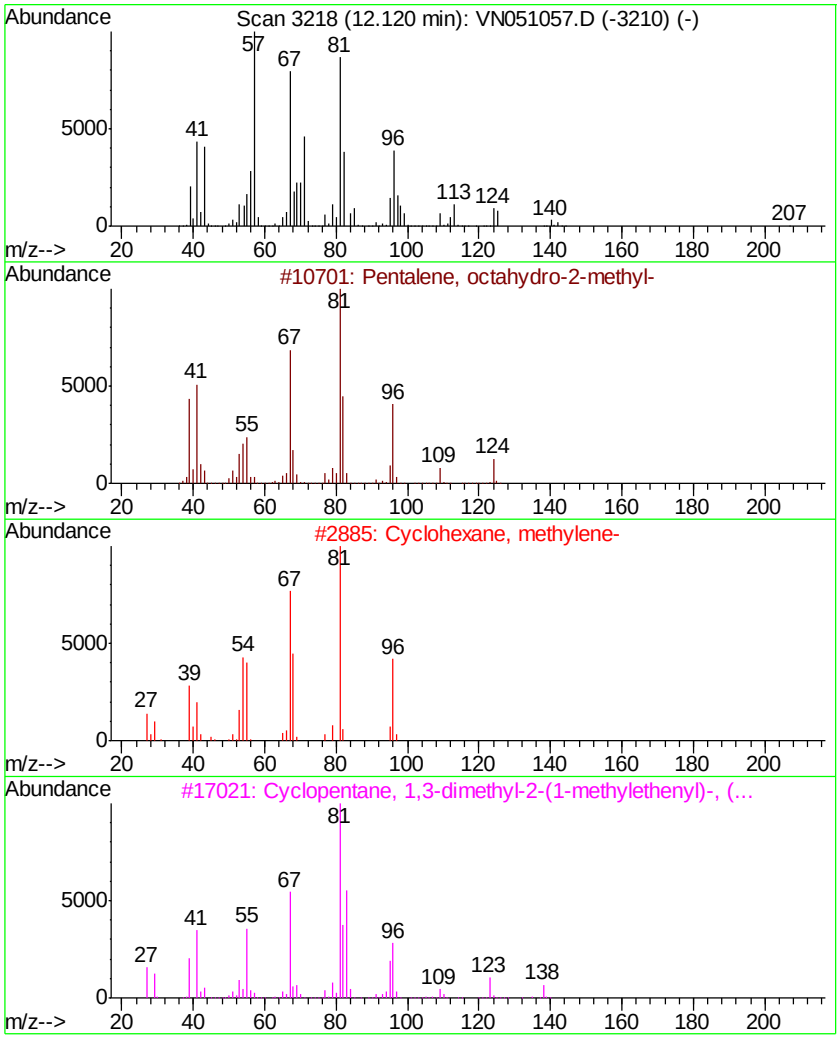
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

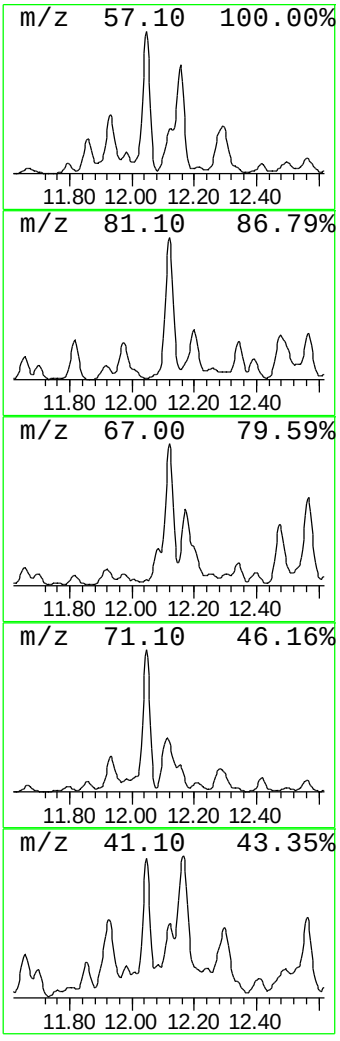
****

Peak Number 6 Pentalene, octahydro-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.12	229.06 ug/l	15313300	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentalene, octahydro-2-methyl-	124	C9H16	003868-64-2	83
2	Cyclohexane, methylene-	96	C7H12	001192-37-6	52
3	Cyclopentane, 1,3-dimethyl-2-(1-...	138	C10H18	061142-31-2	50
4	1H-Indene, octahydro-, trans-	124	C9H16	003296-50-2	49
5	Bicyclo[3.3.1]nonane	124	C9H16	000280-65-9	43





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ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : EP1-MW-D(10-15)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N082118W.M
Quant Title : SW846 8260

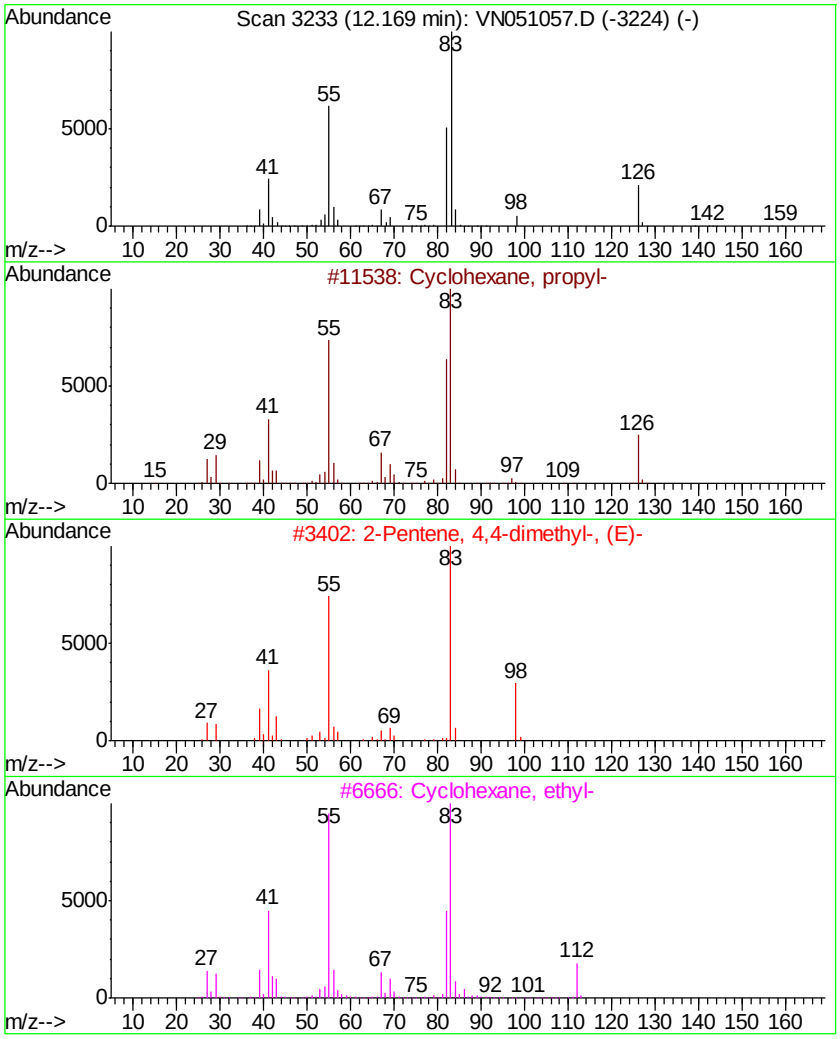
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

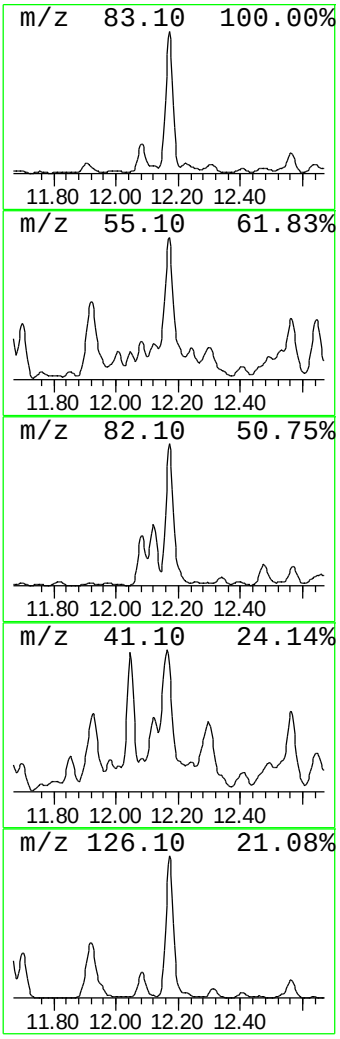
****

Peak Number 7 Cyclohexane, propyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.17	490.53 ug/l	32793100	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, propyl-	126	C9H18	001678-92-8	87
2	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	52
3	Cyclohexane, ethyl-	112	C8H16	001678-91-7	50
4	2-Pyrazoline, 1-methyl-4-propyl-	126	C7H14N2	033063-77-3	50
5	1-Butene, 2,3,3-trimethyl-	98	C7H14	000594-56-9	50





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN090718\
Data File : VN051057.D
Acq On : 7 Sep 2018 16:40
Operator : MD\SY
Sample : J4693-15 5X
Misc : 5.51g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : EP1-MW-D(10-15)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N082118W.M
Quant Title : SW846 8260

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

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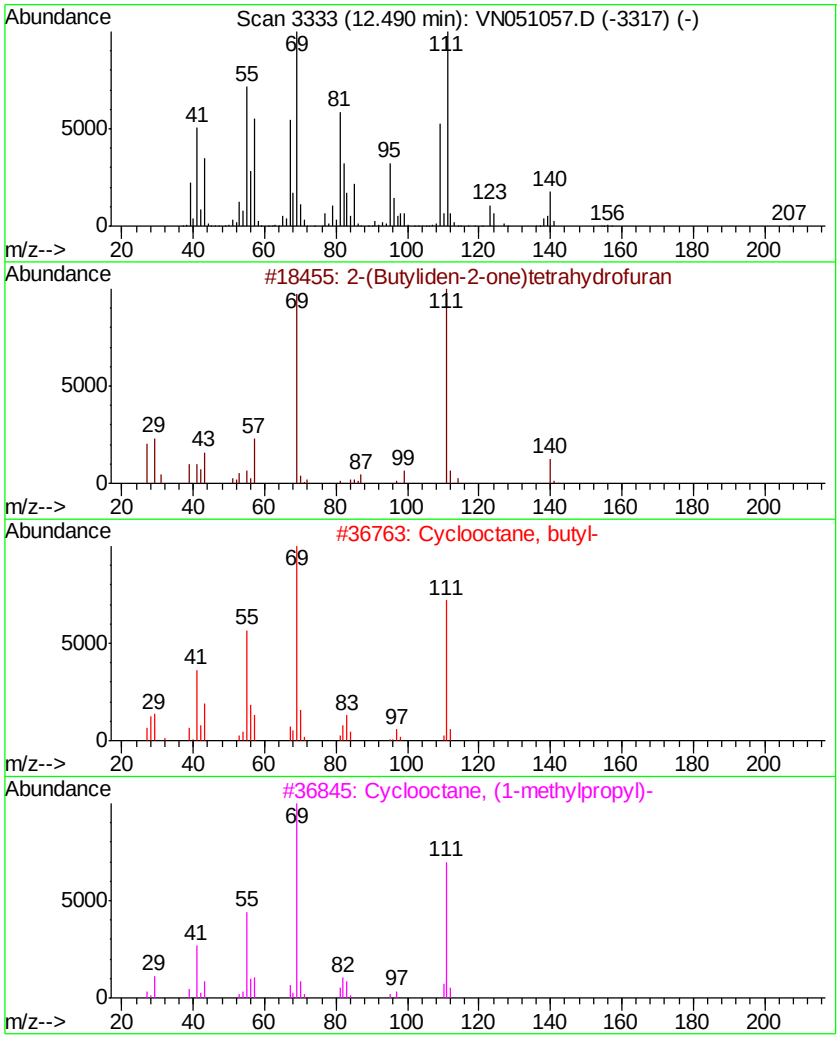
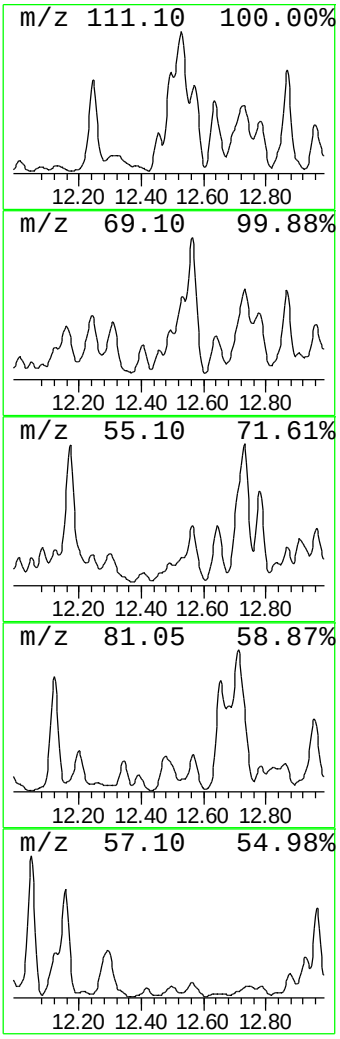
Peak Number 8 unknown12.49 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.49	91.04 ug/l	13516700	1,4-Dichlorobenzene-d4	13.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(Butyliden-2-one)tetrahydrofuran	140	C8H12O2	343270-50-8	43
2	Cyclooctane, butyl-	168	C12H24	016538-93-5	38
3	Cyclooctane, (1-methylpropyl)-	168	C12H24	016538-89-9	38
4	Cyclohexane, 1,3-dimethyl-2-meth...	124	C9H16	019781-47-6	30
5	Cyclohexene, 3,3,5-trimethyl-	124	C9H16	000503-45-7	25





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN090718\
Data File : VN051057.D
Acq On : 7 Sep 2018 16:40
Operator : MD\SY
Sample : J4693-15 5X
Misc : 5.51g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : EP1-MW-D(10-15)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N082118W.M
Quant Title : SW846 8260

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

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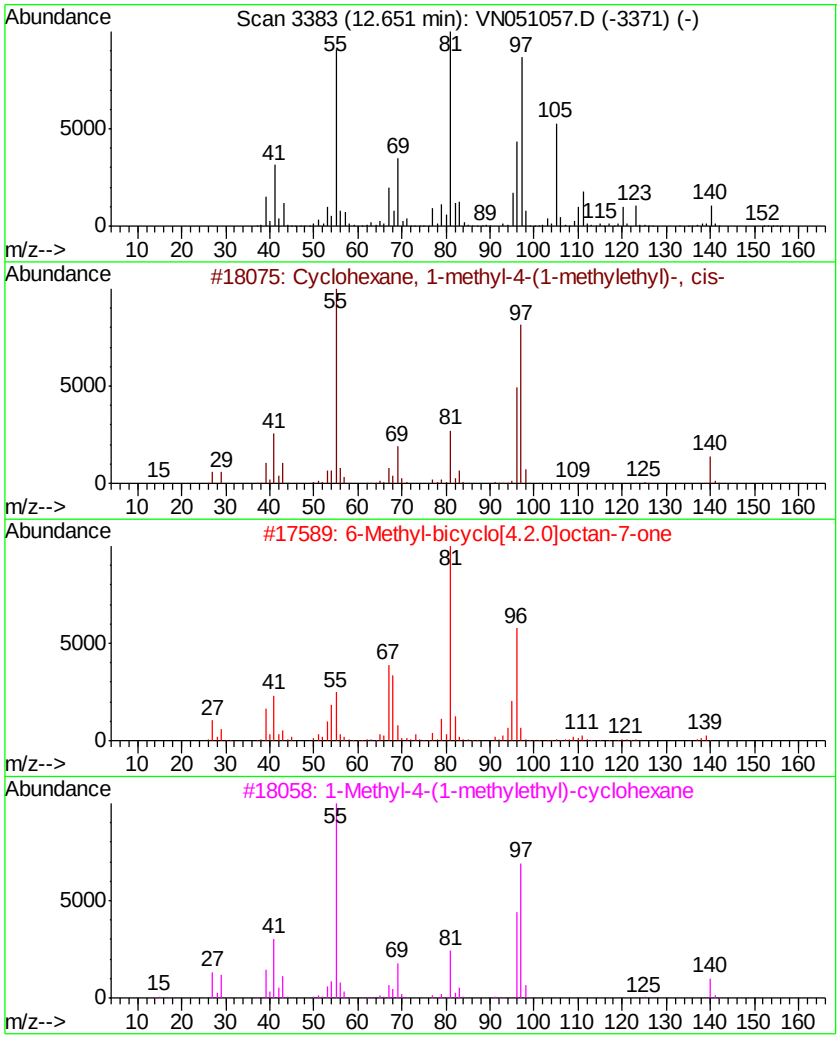
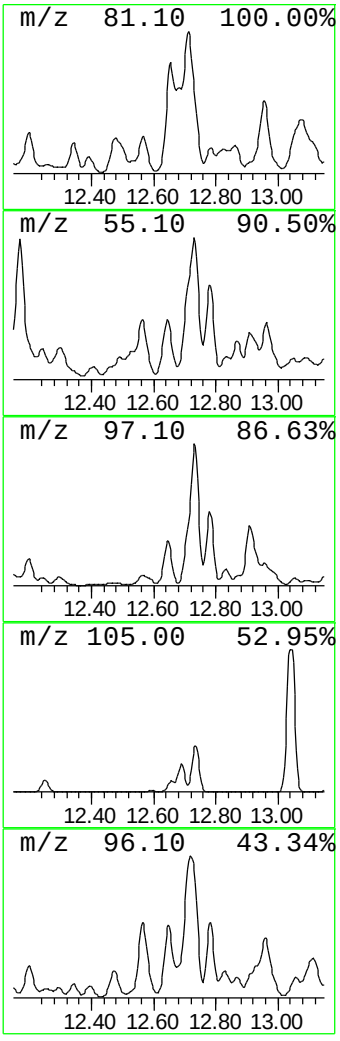
Peak Number 9 unknown12.65 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.65	103.08 ug/l	15303500	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	45
2	6-Methyl-bicyclo[4.2.0]octan-7-one	138	C9H14O	1000193-87-2	43
3	1-Methyl-4-(1-methylethyl)-cyclo...	140	C10H20	000099-82-1	43
4	Cyclohexane, 1-methyl-4-(1-methy...	140	C10H20	001678-82-6	43
5	m-Menthane, (1S,3S)-(+)-	140	C10H20	013837-67-7	43





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN090718\
Data File : VN051057.D
Acq On : 7 Sep 2018 16:40
Operator : MD\SY
Sample : J4693-15 5X
Misc : 5.51g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : EP1-MW-D(10-15)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N082118W.M
Quant Title : SW846 8260

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

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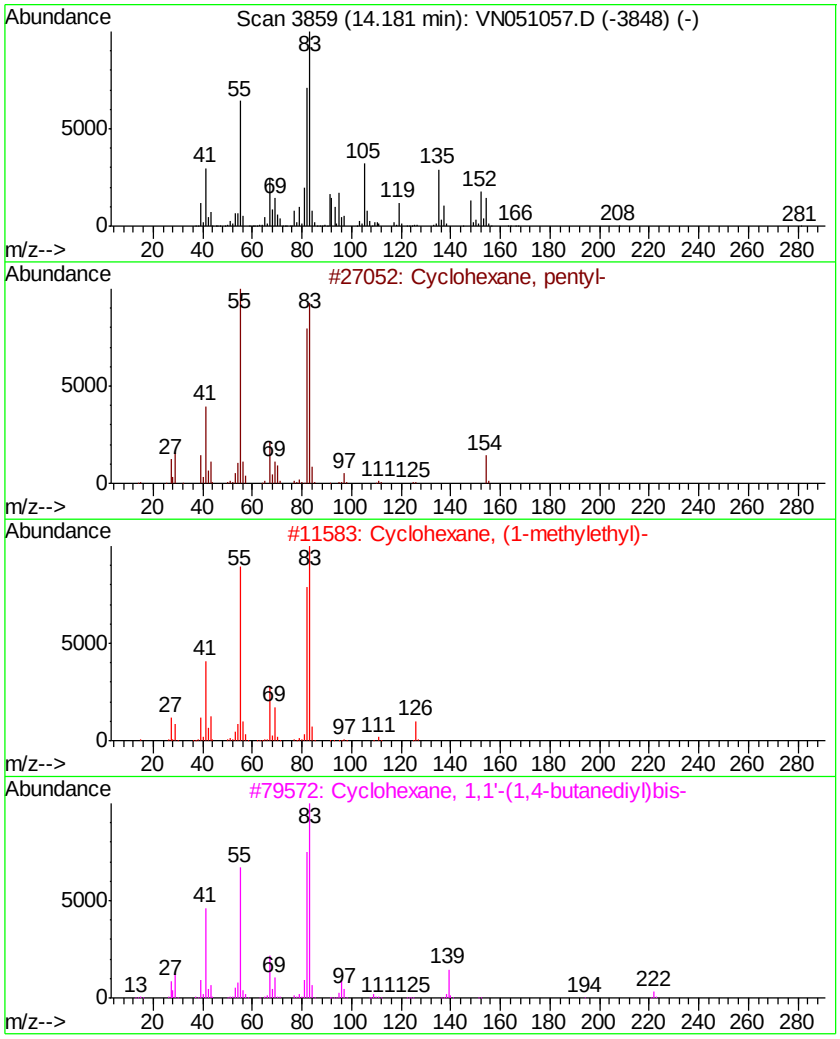
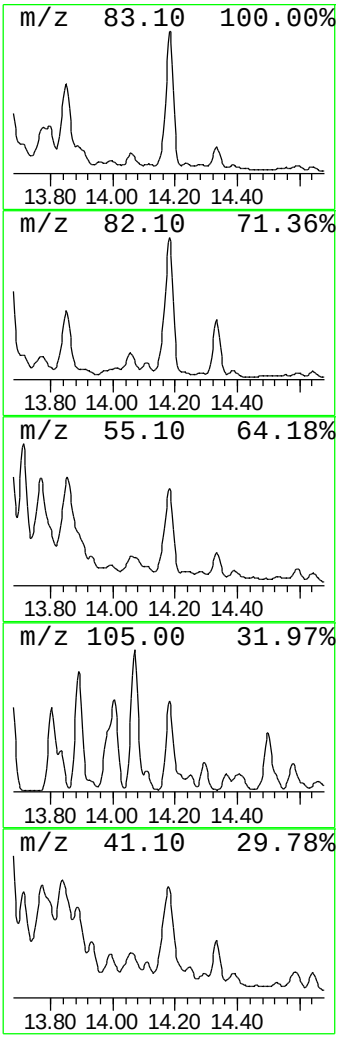
Peak Number 10 Cyclohexane, pentyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.18	66.70 ug/l	9901880	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	Cyclohexane, (1-methylethyl)-	126	C9H18	000696-29-7	46
3	Cyclohexane, 1,1'-(1,4-butanediy...	222	C16H30	006165-44-2	43
4	3-Cyclohexyl-1-chloropropane	160	C9H17Cl	001124-62-5	43
5	1,6-Octadiene, 5,7-dimethyl-, (R)-	138	C10H18	085006-04-8	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN090718\
Data File : VN051057.D
Acq On : 7 Sep 2018 16:40
Operator : MD\SY
Sample : J4693-15 5X
Misc : 5.51g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : EP1-MW-D(10-15)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N082118W.M
Quant Title : SW846 8260

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Cyclohexane, 1,1,...	11.00	67.6	ug/l	4516640	3	11.41	3342650	50.0
Cyclohexane, 1-et...	11.70	117.7	ug/l	7869880	3	11.41	3342650	50.0
Hexane, 2,4-dimet...	11.85	84.7	ug/l	5660730	3	11.41	3342650	50.0
Octane, 3,6-dimet...	12.05	294.3	ug/l	19672700	3	11.41	3342650	50.0
Pentalene, octahy...	12.12	229.1	ug/l	15313300	3	11.41	3342650	50.0
Cyclohexane, propyl-	12.17	490.5	ug/l	32793100	3	11.41	3342650	50.0
unknown12.49	12.49	91.0	ug/l	13516700	4	13.35	7423210	50.0
unknown12.65	12.65	103.1	ug/l	15303500	4	13.35	7423210	50.0
Cyclohexane, pentyl-	14.18	66.7	ug/l	9901880	4	13.35	7423210	50.0