LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA N\Data\VN050219\
Data File : VN055371.D
Acq On : 3 May 2019 1:57
Operator : JC/SP
Sample : K2658-12 10X
Misc : 6.07g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : EP1-SB-E2-3(17-20)

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\82N042919W.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	301174	768592	2.02%	0.237%
2	7.667	1821	1833	1855	rVB	517567	1235917	3.25%	0.381%
3	8.027	1928	1945	1971	rBV	338452	804679	2.11%	0.248%
4	8.587	2104	2119	2142	rBV	820928	1777961	4.67%	0.548%
5	10.091	2572	2587	2615	rBV2	1526331	3280010	8.62%	1.011%
6	10.432	2661	2693	2709	rBV3	266226	589672	1.55%	0.182%
7	10.718	2771	2782	2793	rVB	413902	706225	1.86%	0.218%
8	10.818	2800	2813	2826	rBV	331753	687297	1.81%	0.212%
9	10.886	2826	2834	2842	rVV3	233201	418188	1.10%	0.129%
10	10.950	2846	2854	2862	rVV	800559	1307303	3.44%	0.403%
11	11.005	2862	2871	2881	rVV2	1292506	2213219	5.82%	0.682%
12	11.124	2896	2908	2916	rBV3	916566	1686592	4.43%	0.520%
13	11.207	2916	2934	2951	rVB5	1516283	4599719	12.09%	1.418%
14	11.297	2951	2962	2983	rBV	2139309	3943557	10.36%	1.215%
15	11.406	2985	2996	3014	rBV	1155486	2497425	6.56%	0.770%
16	11.509	3015	3028	3032	rBV3	686743	1317309	3.46%	0.406%
17	11.541	3033	3038	3044	rVV	860626	1188477	3.12%	0.366%
18	11.615	3045	3061	3066	rVV5	3298048	7939780	20.87%	2.447%
19	11.654	3067	3073	3081	rVV2	4729485	8611152	22.63%	2.654%
20	11.696	3081	3086	3097	rVB3	3067762	4992321	13.12%	1.539%
21	11.757	3097	3105	3111	rBV3	584009	1023828	2.69%	0.316%
22	11.850	3128	3134	3142	rVB3	1157096	1716849	4.51%	0.529%
23	11.921	3142	3156	3169	rBV6	5679562	14368567	37.76%	4.429%
24	12.043	3187	3194	3201	rBV	4458717	5928848	15.58%	1.827%
25	12.082	3202	3206	3209	rVV2	971556	1020507	2.68%	0.315%
26	12.120	3210	3218	3223	rVV2	5021912	8412686	22.11%	2.593%
27	12.165	3224	3232	3249	rVB5	9263368	18658713	49.04%	5.751%
28	12.297	3266	3273	3279	rBV5	2184754	3826203	10.06%	1.179%
29	12.336	3280	3285	3295	rVB2	5740131	8757395	23.02%	2.699%
30	12.403	3296	3306	3315	rBV6	2168227	4252099	11.17%	1.311%
31	12.484	3316	3331	3339	rBV6	1912735	5724087	15.04%	1.764%
32	12.561	3348	3355	3371	rVB3	6954126	15642586	41.11%	4.821%
33	12.654	3372	3384	3391	rBV2	10628596	19993254	52.54%	6.162%
34	12.731	3402	3408	3417	rVB2	14738668	23263688	61.14%	7.170%

LSC Area Percent Report

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Acq On : 3 May 2019 1:57
Operator : JC/SP
Sample : K2658-12 10X
Misc : 6.07g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : EP1-SB-E2-3(17-20)

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\82N042919W.M
Title : SW846 8260

35	12.779	3418	3423	3433	rVB3	3774666	5790987	15.22%	1.785%
36	12.869	3444	3451	3457	rBV6	1924516	3139002	8.25%	0.968%
37	12.959	3472	3479	3493	rVB3	5830101	10603527	27.87%	3.268%
38	13.040	3493	3504	3514	rBV	23600465	38050539	100.00%	11.728%
39	13.168	3533	3544	3552	rVB6	2522298	4991462	13.12%	1.538%
40	13.239	3553	3566	3574	rVV5	5963032	11638562	30.59%	3.587%
41	13.287	3575	3581	3589	rVB2	2697309	3890982	10.23%	1.199%
42	13.374	3599	3608	3623	rVB	9313514	15195389	39.93%	4.684%
43	13.512	3646	3651	3655	rBV	917187	1161301	3.05%	0.358%
44	13.583	3666	3673	3688	rVB4	4672135	9255392	24.32%	2.853%
45	13.660	3688	3697	3708	rVB2	4573899	7773085	20.43%	2.396%
46	13.802	3734	3741	3745	rBV	1795334	2635298	6.93%	0.812%
47	13.831	3746	3750	3759	rVV	2618361	3737055	9.82%	1.152%
48	13.885	3760	3767	3777	rVB	3323969	5164799	13.57%	1.592%
49	13.992	3791	3800	3809	rVB4	2610092	4230258	11.12%	1.304%
50	14.046	3810	3817	3821	rBV3	598513	943212	2.48%	0.291%
51	14.127	3834	3842	3849	rBV2	998965	1509262	3.97%	0.465%
52	14.175	3849	3857	3862	rBV5	928141	1657524	4.36%	0.511%
53	14.249	3874	3880	3887	rVB	1467315	2038486	5.36%	0.628%
54	14.294	3887	3894	3899	rBV3	717606	961142	2.53%	0.296%
55	14.332	3900	3906	3913	rVB	891771	1190663	3.13%	0.367%
56	14.477	3944	3951	3959	rBV3	258087	495329	1.30%	0.153%
57	14.522	3960	3965	3973	rVB3	408805	570913	1.50%	0.176%
58	14.580	3973	3983	3996	rBV2	1611988	3075027	8.08%	0.948%
59	14.644	3997	4003	4013	rVB3	278068	420104	1.10%	0.129%
60	14.953	4092	4099	4118	rVB5	210265	470748	1.24%	0.145%
61	15.130	4146	4154	4177	rVB	349179	696955	1.83%	0.215%

Sum of corrected areas: 324441708

LSC Report - Integrated Chromatogram

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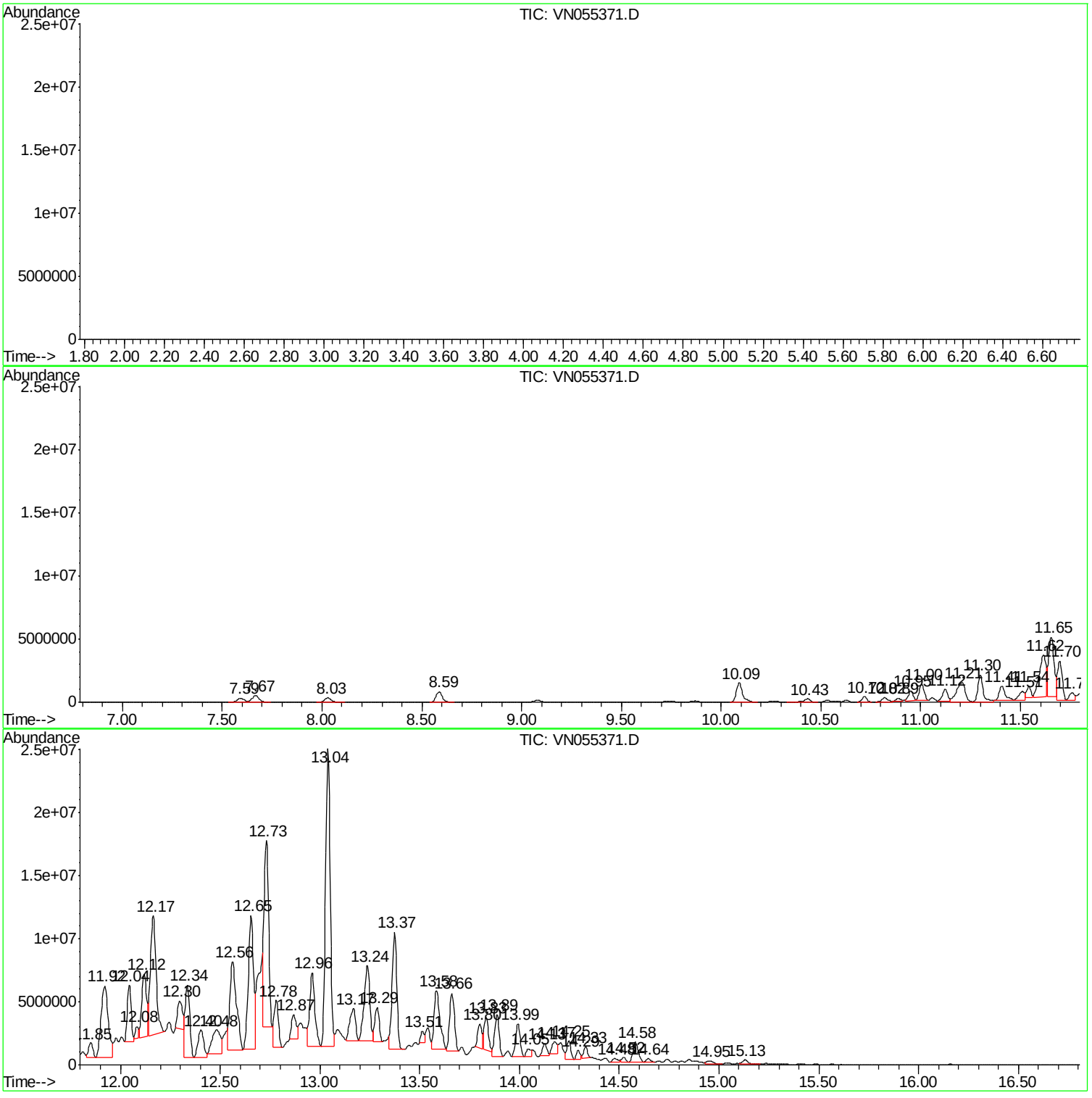
Misc : 6.07g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
EP1-SB-E2-3(17-20)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N042919W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN050219\
Data File : VN055371.D
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Operator : JC/SP
Sample : K2658-12 10X
Misc : 6.07g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : EP1-SB-E2-3(17-20)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N042919W.M
Quant Title : SW846 8260

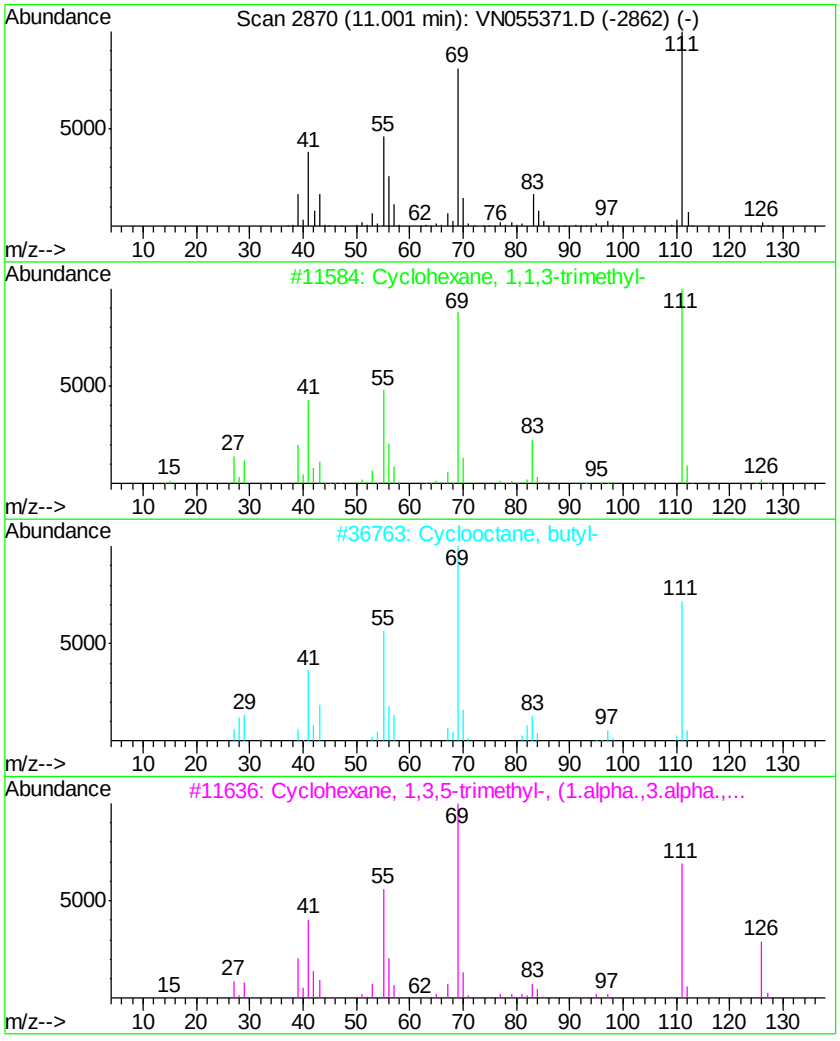
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

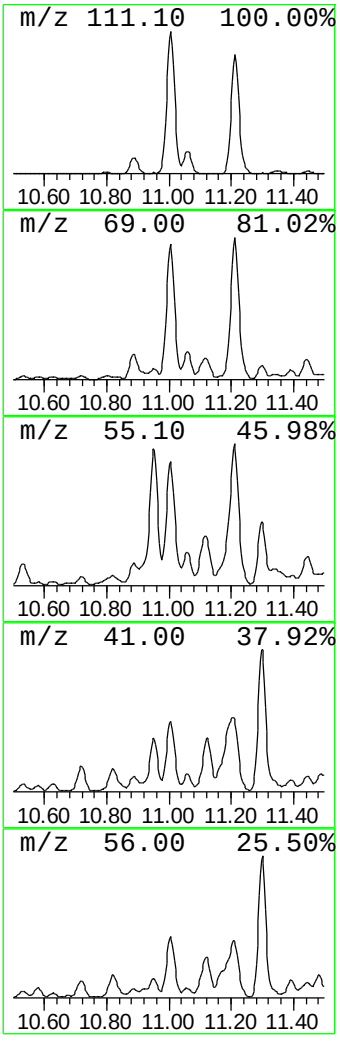
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.00	44.31 ug/l	2213220	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,1,3-trimethyl-	126	C9H18	003073-66-3	91
2	Cyclooctane, butyl-	168	C12H24	016538-93-5	78
3	Cyclohexane, 1,3,5-trimethyl-, (...	126	C9H18	001795-26-2	78
4	Cyclohexane, 1,3,5-trimethyl-	126	C9H18	001839-63-0	72
5	Cyclooctane, (1-methylpropyl)-	168	C12H24	016538-89-9	59





Data Path : Z:\voasrv\HPCHEM1\MSVOA N\Data\VN050219\
Data File : VN055371.D
Acq On : 3 May 2019 1:57
Operator : JC/SP
Sample : K2658-12 10X
Misc : 6.07g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : EP1-SB-E2-3(17-20)

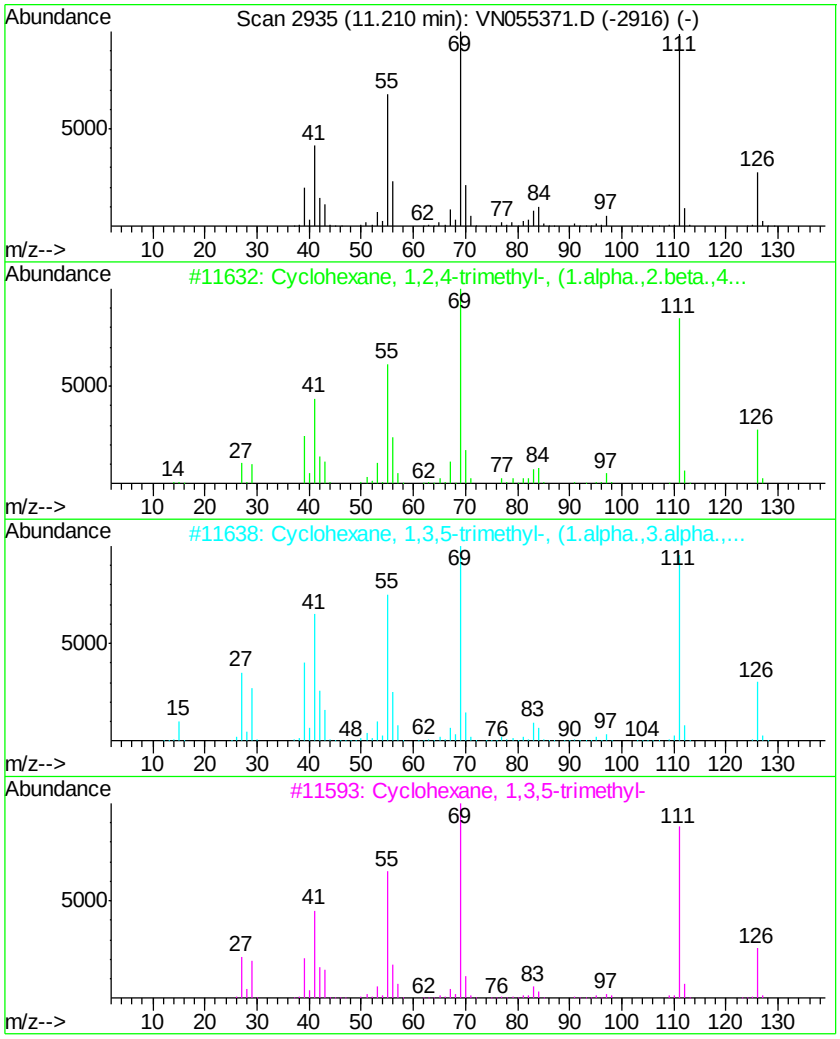
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N042919W.M
Quant Title : SW846 8260

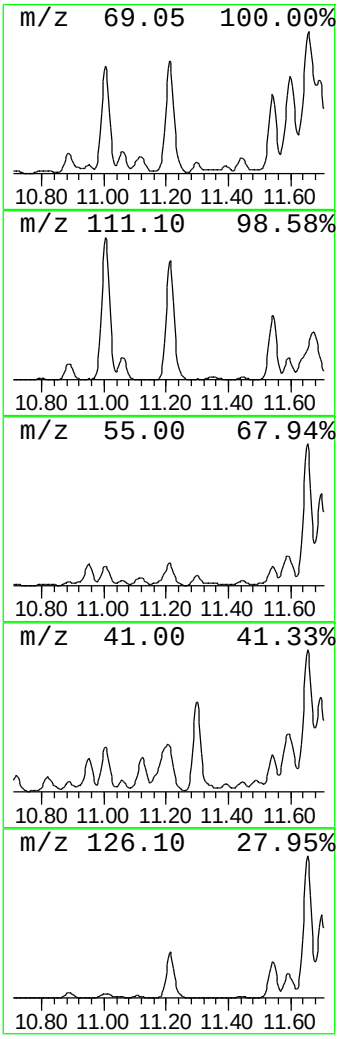
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Cyclohexane, 1,2,4-trimethy... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.21	92.09 ug/l	4599720	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,2,4-trimethyl-, (...	126	C9H18	007667-60-9	95
2	Cyclohexane, 1,3,5-trimethyl-, (...	126	C9H18	001795-26-2	87
3	Cyclohexane, 1,3,5-trimethyl-	126	C9H18	001839-63-0	83
4	Cyclohexane, 1,2,4-trimethyl-	126	C9H18	002234-75-5	76
5	Cyclohexane, 1,3,5-trimethyl-, (...	126	C9H18	001795-27-3	74





Library Search Compound Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA N\Data\VN050219\
Data File : VN055371.D
Acq On : 3 May 2019 1:57
Operator : JC/SP
Sample : K2658-12 10X
Misc : 6.07g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : EP1-SB-E2-3(17-20)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N042919W.M
Quant Title : SW846 8260

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

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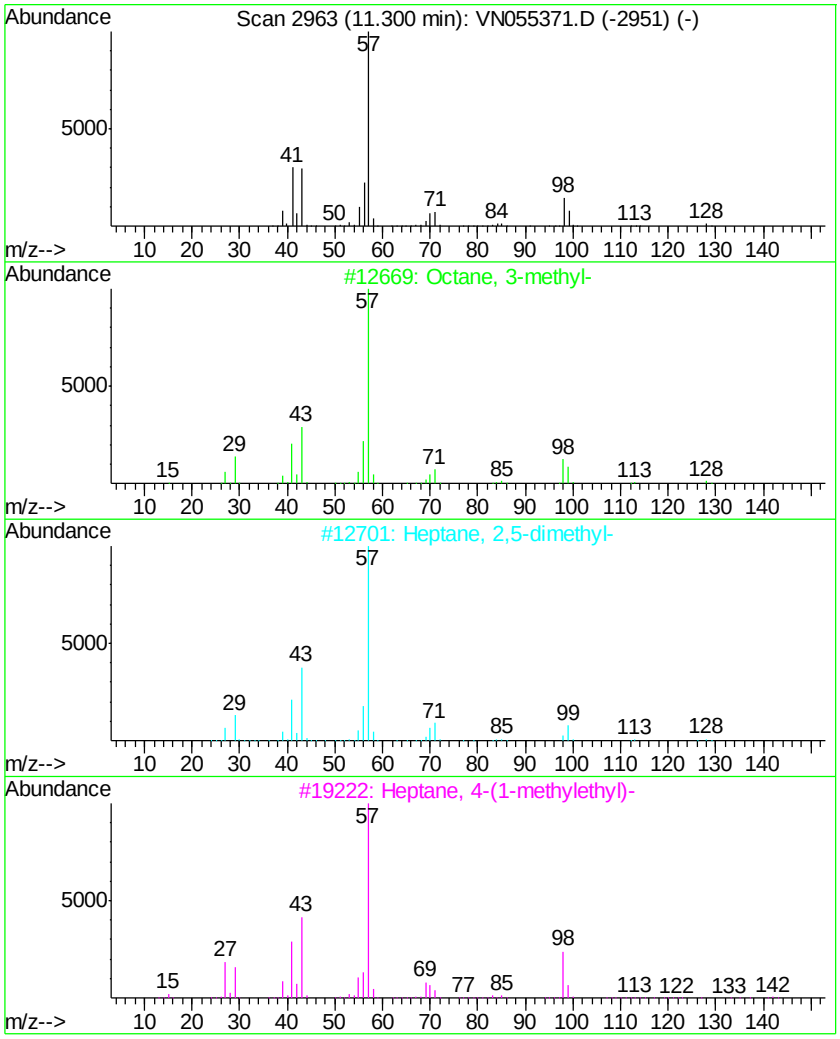
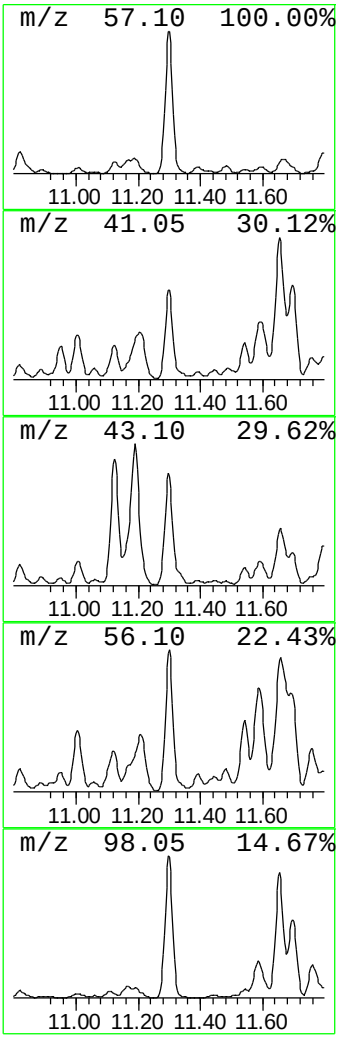
Peak Number 3 Octane, 3-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.30	78.95 ug/l	3943560	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 3-methyl-	128	C9H20	002216-33-3	91
2	Heptane, 2,5-dimethyl-	128	C9H20	002216-30-0	64
3	Heptane, 4-(1-methylethyl)-	142	C10H22	052896-87-4	64
4	Oxalic acid, isobutyl heptyl ester	244	C13H24O4	1000309-37-2	59
5	2,2,4,4-Tetramethyloctane	170	C12H26	062183-79-3	59





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN050219\
Data File : VN055371.D
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Operator : JC/SP
Sample : K2658-12 10X
Misc : 6.07g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : EP1-SB-E2-3(17-20)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N042919W.M
Quant Title : SW846 8260

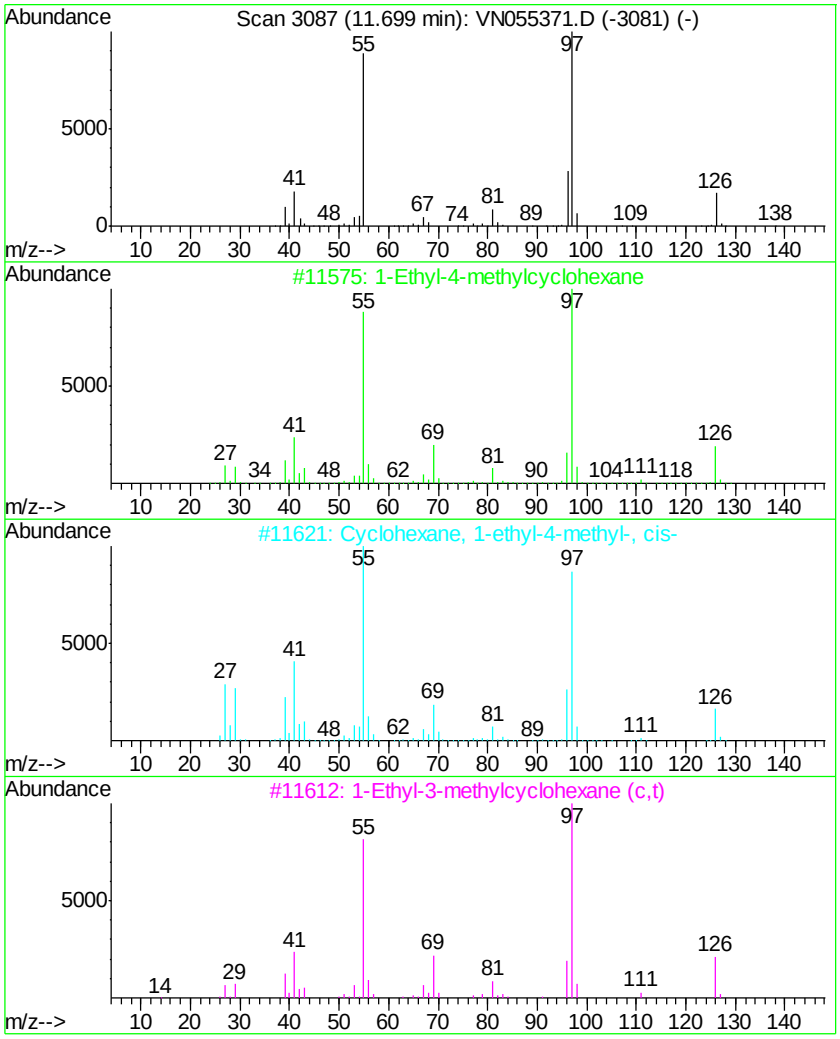
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

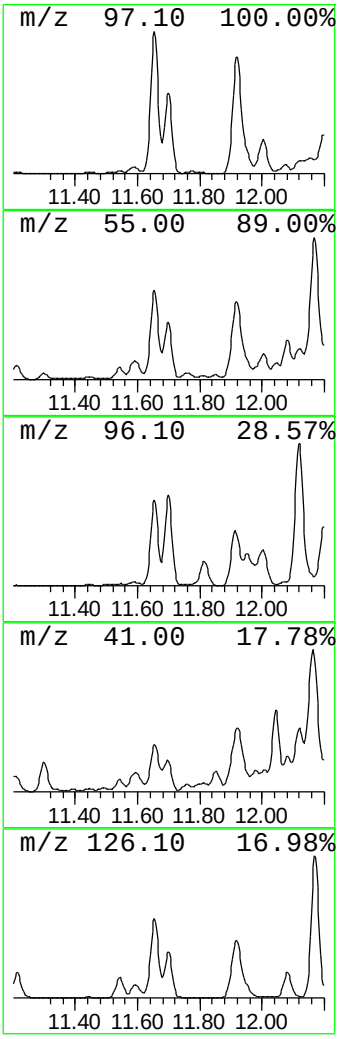
****

Peak Number 4 1-Ethyl-4-methylcyclohexane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.70	99.95 ug/l	4992320	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Ethyl-4-methylcyclohexane	126	C9H18	003728-56-1	87
2	Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	004926-78-7	83
3	1-Ethyl-3-methylcyclohexane (c,t)	126	C9H18	003728-55-0	78
4	Cyclohexane, 1-ethyl-1-methyl-	126	C9H18	004926-90-3	72
5	3,5-Dimethyl-3-heptene	126	C9H18	059643-68-4	64





Library Search Compound Report

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Misc : 6.07g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : EP1-SB-E2-3(17-20)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N042919W.M
Quant Title : SW846 8260

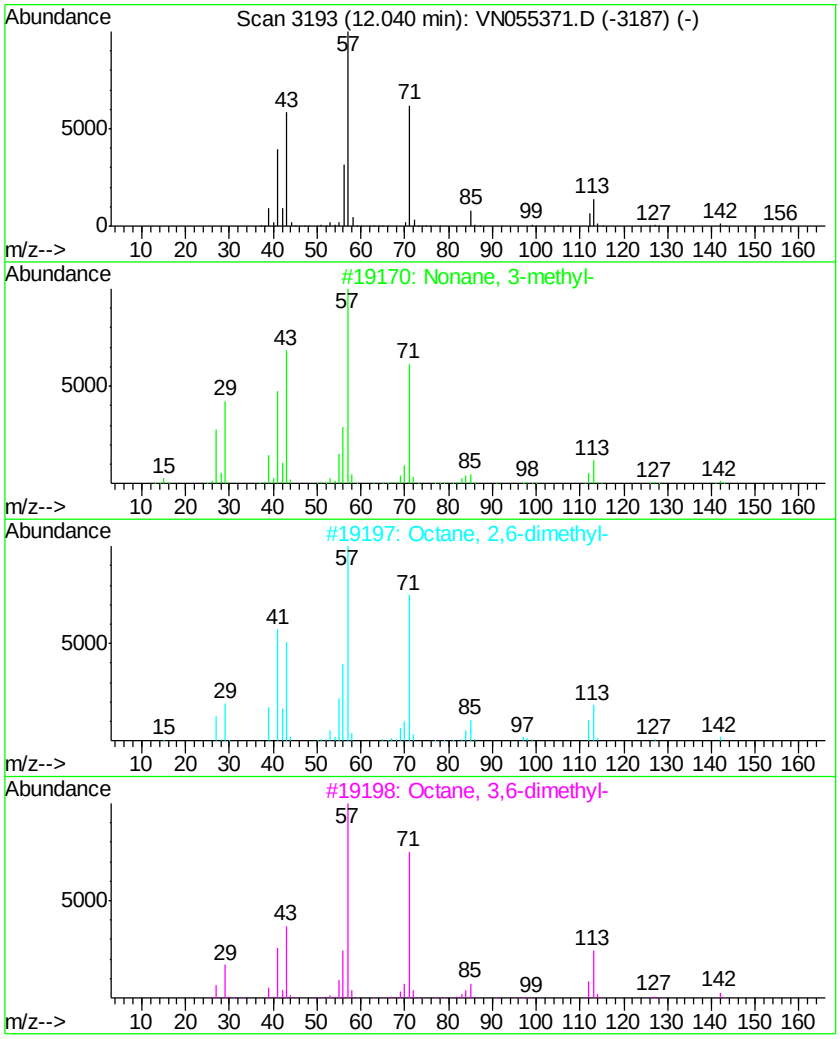
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

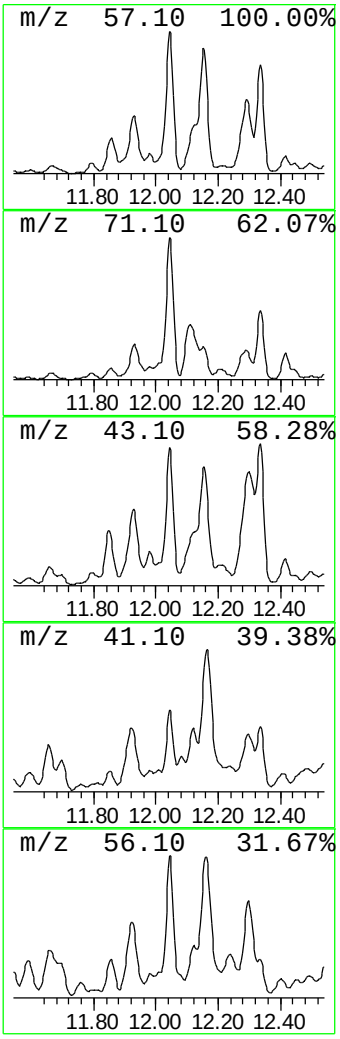
****

Peak Number 5 Nonane, 3-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.04	118.70 ug/l	5928850	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	90
4	Sulfurous acid, 2-ethylhexyl non...	320	C17H36O3S	1000309-19-2	64
5	Decane, 2,6,7-trimethyl-	184	C13H28	062108-25-2	64





Library Search Compound Report

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Misc : 6.07g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : EP1-SB-E2-3(17-20)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N042919W.M
Quant Title : SW846 8260

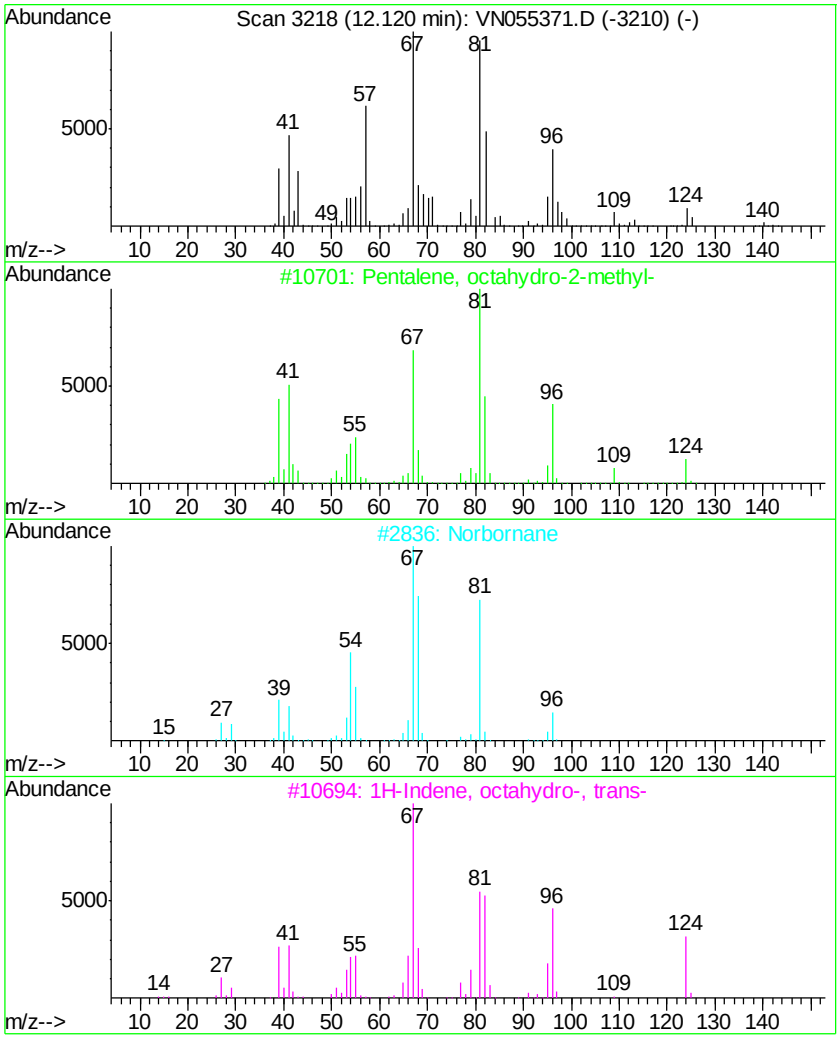
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

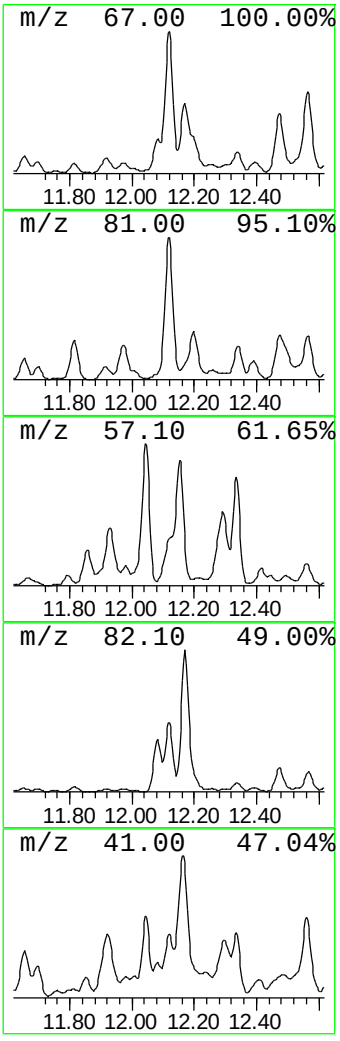
****

Peak Number 6 Pentalene, octahydro-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.12	168.43 ug/l	8412690	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentalene, octahydro-2-methyl-	124	C9H16	003868-64-2	64
2	Norbornane	96	C7H12	000279-23-2	58
3	1H-Indene, octahydro-, trans-	124	C9H16	003296-50-2	58
4	Cyclohexene, 4-methyl-	96	C7H12	000591-47-9	46
5	Cyclohexene, 1-methyl-	96	C7H12	000591-49-1	46





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN050219\
Data File : VN055371.D
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Operator : JC/SP
Sample : K2658-12 10X
Misc : 6.07g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : EP1-SB-E2-3(17-20)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N042919W.M
Quant Title : SW846 8260

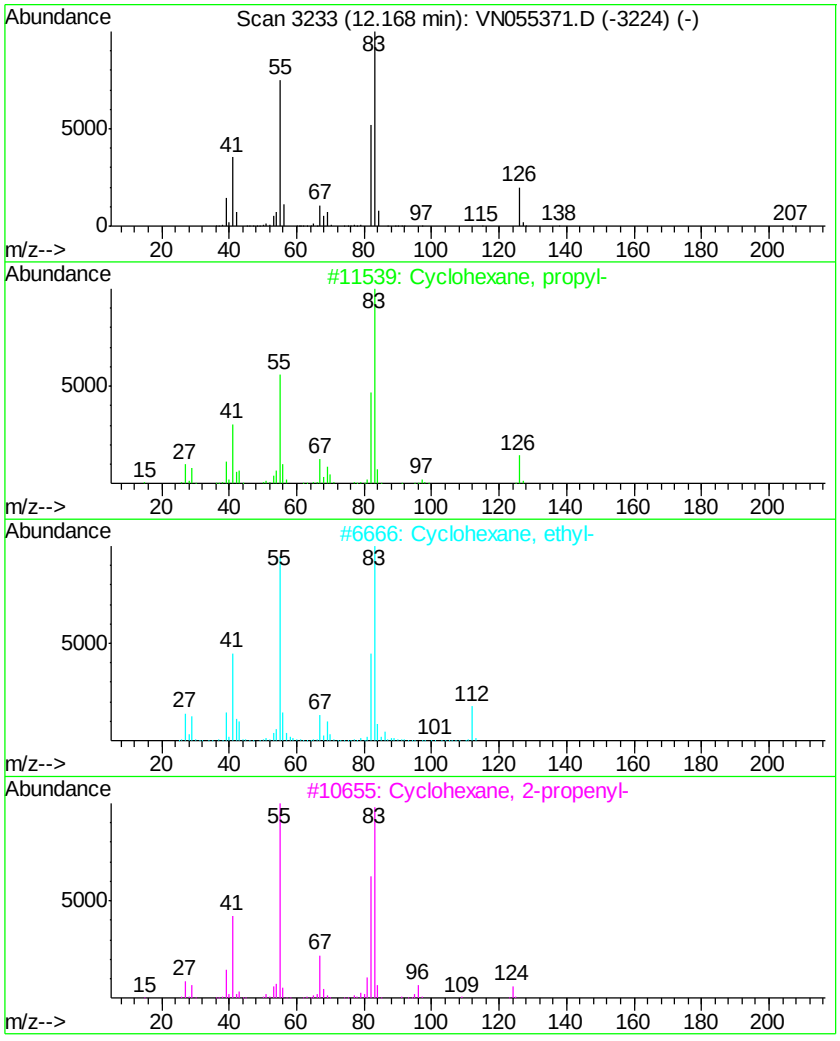
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

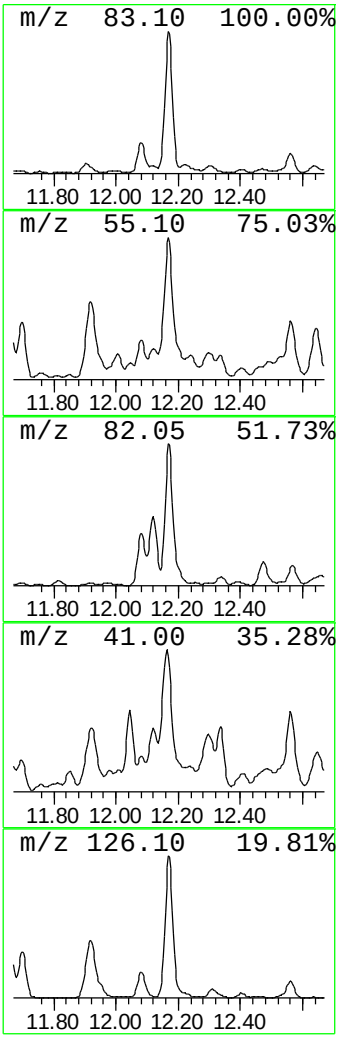
****

Peak Number 7 Cyclohexane, propyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.17	373.56 ug/l	18658700	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, propyl-	126	C9H18	001678-92-8	90
2	Cyclohexane, ethyl-	112	C8H16	001678-91-7	72
3	Cyclohexane, 2-propenyl-	124	C9H16	002114-42-3	59
4	Ethanone, 1-(1-methylcyclopentyl)-	126	C8H14O	013388-93-7	59
5	Cyclopentane, 1-ethyl-1-methyl-	112	C8H16	016747-50-5	59





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN050219\
Data File : VN055371.D
Acq On : 3 May 2019 1:57
Operator : JC/SP
Sample : K2658-12 10X
Misc : 6.07g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : EP1-SB-E2-3(17-20)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N042919W.M
Quant Title : SW846 8260

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

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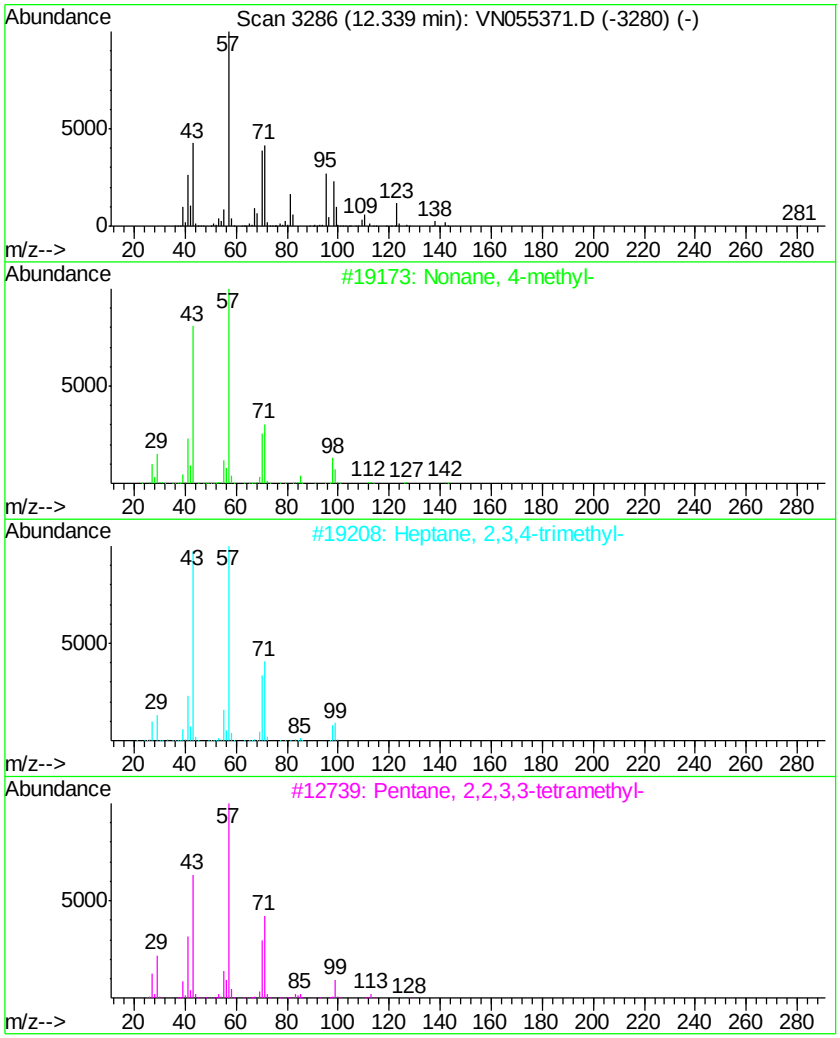
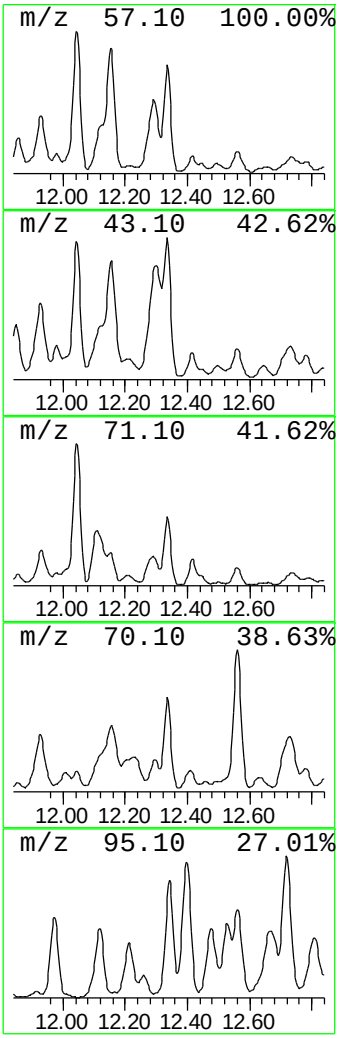
Peak Number 8 Nonane, 4-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.34	175.33 ug/l	8757400	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonane, 4-methyl-	142	C10H22	017301-94-9	64
2	Heptane, 2,3,4-trimethyl-	142	C10H22	052896-95-4	50
3	Pentane, 2,2,3,3-tetramethyl-	128	C9H20	007154-79-2	47
4	Undecane, 4,5-dimethyl-	184	C13H28	017312-79-7	43
5	Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	27





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN050219\
Data File : VN055371.D
Acq On : 3 May 2019 1:57
Operator : JC/SP
Sample : K2658-12 10X
Misc : 6.07g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : EP1-SB-E2-3(17-20)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N042919W.M
Quant Title : SW846 8260

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

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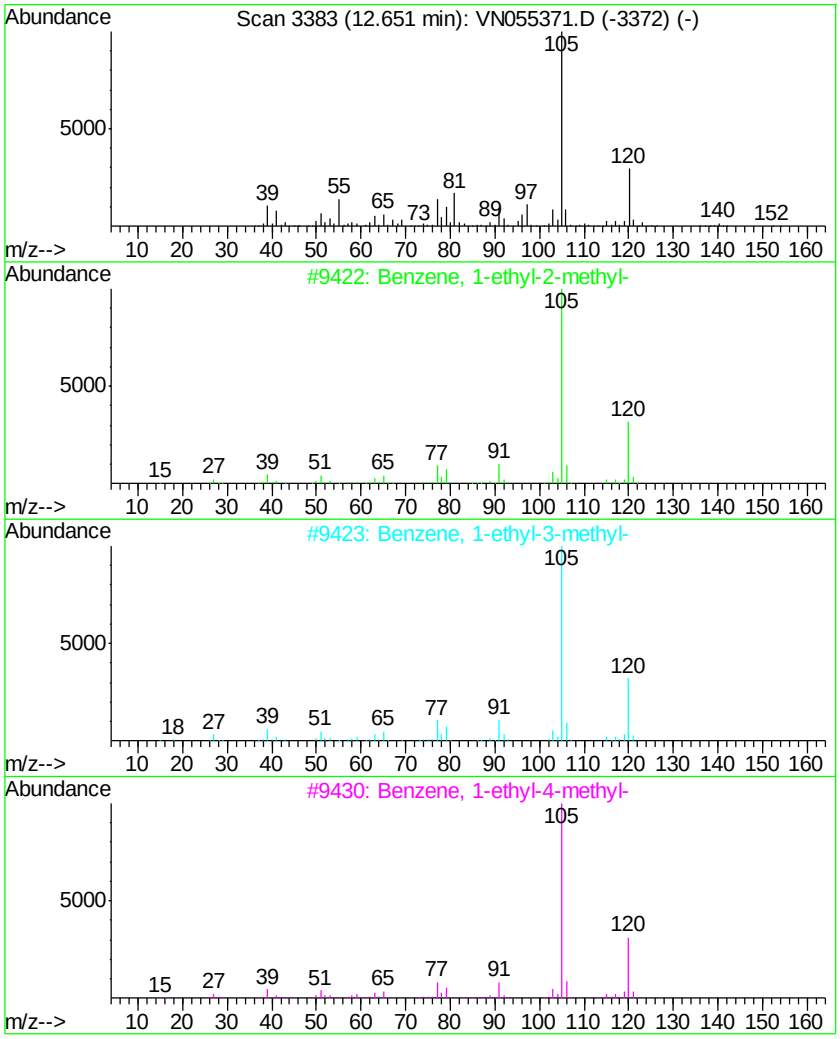
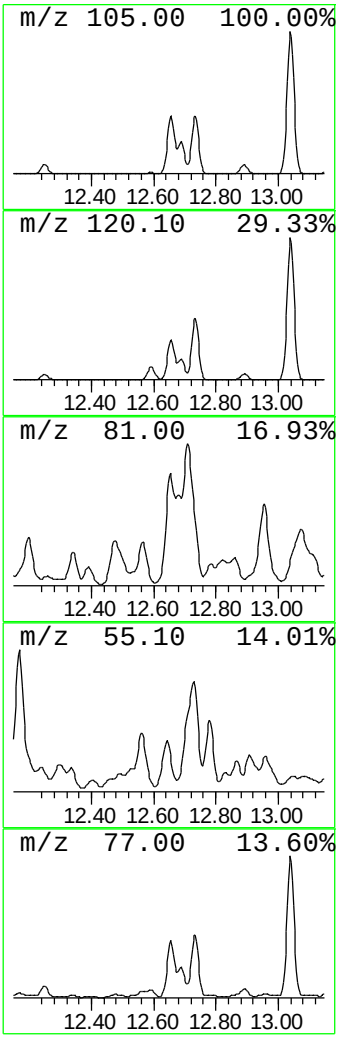
Peak Number 9 Benzene, 1-ethyl-2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.65	65.79 ug/l	19993300	1,4-Dichlorobenzene-d4	13.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	94
3	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	76
4	Mesitylene	120	C9H12	000108-67-8	76
5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	76





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN050219\
Data File : VN055371.D
Acq On : 3 May 2019 1:57
Operator : JC/SP
Sample : K2658-12 10X
Misc : 6.07g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : EP1-SB-E2-3(17-20)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N042919W.M
Quant Title : SW846 8260

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

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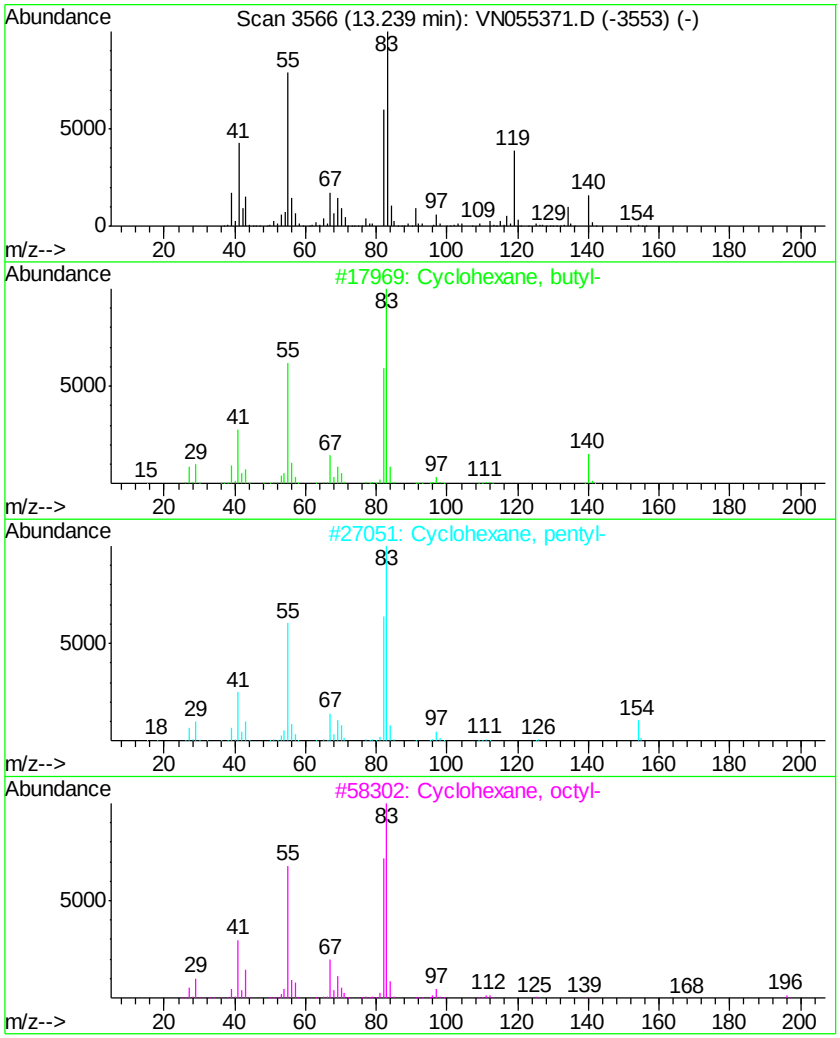
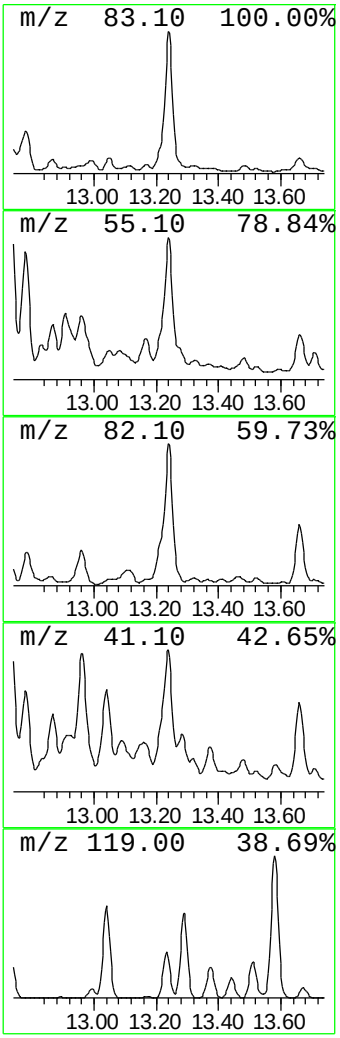
Peak Number 10 Cyclohexane, butyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.24	38.30 ug/l	11638600	1,4-Dichlorobenzene-d4	13.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, butyl-	140	C10H20	001678-93-9	93
2	Cyclohexane, pentyl-	154	C11H22	004292-92-6	64
3	Cyclohexane, octyl-	196	C14H28	001795-15-9	52
4	Cyclohexane, ethyl-	112	C8H16	001678-91-7	52
5	Cyclohexane, undecyl-	238	C17H34	054105-66-7	50





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN050219\
Data File : VN055371.D
Acq On : 3 May 2019 1:57
Operator : JC/SP
Sample : K2658-12 10X
Misc : 6.07g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : EP1-SB-E2-3(17-20)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N042919W.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	44.3	ug/l	2213220	3	11.41	2497430	50.0
Cyclohexane, 1,2,...	11.21	92.1	ug/l	4599720	3	11.41	2497430	50.0
Octane, 3-methyl-	11.30	79.0	ug/l	3943560	3	11.41	2497430	50.0
1-Ethyl-4-methylc...	11.70	100.0	ug/l	4992320	3	11.41	2497430	50.0
Nonane, 3-methyl-	12.04	118.7	ug/l	5928850	3	11.41	2497430	50.0
Pentalene, octahy...	12.12	168.4	ug/l	8412690	3	11.41	2497430	50.0
Cyclohexane, propyl-	12.17	373.6	ug/l	18658700	3	11.41	2497430	50.0
Nonane, 4-methyl-	12.34	175.3	ug/l	8757400	3	11.41	2497430	50.0
Benzene, 1-ethyl-...	12.65	65.8	ug/l	19993300	4	13.34	15195400	50.0
Cyclohexane, butyl-	13.24	38.3	ug/l	11638600	4	13.34	15195400	50.0