LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA N\Data\VN052319\
Data File : VN055769.D
Acq On : 23 May 2019 21:47
Operator : JC/SP
Sample : K2976-04
Misc : 6.67g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 32 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : EP1-SB-E3-4R(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\82N052319W.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	3.358	473	493	516	rBV3	109102	468718	6.54%	0.663%
2	7.587	1788	1808	1819	rBV	211220	523548	7.30%	0.740%
3	7.661	1819	1831	1861	rVB	384472	929953	12.97%	1.315%
4	8.024	1926	1944	1973	rBV	209163	484202	6.75%	0.685%
5	8.583	2103	2118	2155	rVB	529941	1138512	15.88%	1.610%
6	10.091	2571	2587	2625	rBV	816397	1575534	21.98%	2.228%
7	11.123	2896	2908	2915	rBV3	56218	98400	1.37%	0.139%
8	11.191	2915	2929	2949	rVB3	95822	270618	3.78%	0.383%
9	11.297	2949	2962	2981	rBV	113253	220871	3.08%	0.312%
10	11.406	2982	2996	3014	rBV	720873	1352206	18.86%	1.912%
11	11.599	3044	3056	3063	rBV5	105725	243933	3.40%	0.345%
12	11.654	3064	3073	3080	rVV	249001	397127	5.54%	0.561%
13	11.696	3081	3086	3096	rVB2	199007	312513	4.36%	0.442%
14	11.757	3096	3105	3110	rBV2	75357	129682	1.81%	0.183%
15	11.792	3111	3116	3124	rBV2	49116	72740	1.01%	0.103%
16	11.850	3125	3134	3143	rBV3	395680	672222	9.38%	0.950%
17	11.924	3143	3157	3168	rBV5	879008	1970152	27.48%	2.786%
18	11.979	3169	3174	3179	rBV	175506	200097	2.79%	0.283%
19	12.043	3185	3194	3203	rVB	1951341	2832380	39.51%	4.005%
20	12.120	3208	3218	3221	rVV4	708020	1164220	16.24%	1.646%
21	12.159	3222	3230	3241	rVB5	1680884	3307864	46.15%	4.677%
22	12.294	3261	3272	3279	rBV5	1156625	2480743	34.61%	3.508%
23	12.336	3280	3285	3295	rVB	1849763	2751952	38.39%	3.891%
24	12.406	3295	3307	3316	rBV5	967593	1922494	26.82%	2.718%
25	12.493	3317	3334	3339	rBV7	534515	1260356	17.58%	1.782%
26	12.561	3348	3355	3369	rVB4	1507508	2954552	41.22%	4.177%
27	12.644	3369	3381	3389	rBV7	983584	2234779	31.18%	3.160%
28	12.728	3393	3407	3416	rVV4	2641816	7168172	100.00%	10.135%
29	12.779	3417	3423	3433	rVB3	1440967	2407441	33.59%	3.404%
30	12.869	3443	3451	3457	rBV5	850103	1255926	17.52%	1.776%
31	12.959	3472	3479	3492	rVB	3357282	5590152	77.99%	7.904%
32	13.040	3493	3504	3512	rBV2	1895900	3352118	46.76%	4.740%
33	13.088	3514	3519	3529	rVB4	550148	777826	10.85%	1.100%
34	13.146	3532	3537	3540	rBV2	332953	409126	5.71%	0.578%

LSC Area Percent Report

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Operator : JC/SP
Sample : K2976-04
Misc : 6.67g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 32 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : EP1-SB-E3-4R(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\82N052319W.M
Title : SW846 8260

35	13.239	3551	3566	3573	rBV3	2106398	4307025	60.09%	6.090%
36	13.593	3669	3676	3687	rBV2	435296	909599	12.69%	1.286%
37	13.660	3688	3697	3707	rVV4	1694450	3206472	44.73%	4.534%
38	13.709	3708	3712	3720	rVB2	447311	606103	8.46%	0.857%
39	13.831	3746	3750	3760	rVB6	758076	1021248	14.25%	1.444%
40	13.885	3761	3767	3776	rVB	1202467	1799460	25.10%	2.544%
41	13.992	3791	3800	3809	rVB4	578532	964105	13.45%	1.363%
42	14.178	3849	3858	3873	rVV7	611661	1620103	22.60%	2.291%
43	14.246	3874	3879	3887	rVB	552483	773466	10.79%	1.094%
44	14.294	3888	3894	3899	rBV3	174936	227776	3.18%	0.322%
45	14.332	3900	3906	3913	rVB3	259894	331480	4.62%	0.469%
46	14.522	3960	3965	3973	rVB3	151722	201928	2.82%	0.286%
47	14.580	3974	3983	3995	rVV2	726730	1400558	19.54%	1.980%
48	14.641	3996	4002	4014	rVB4	242870	425874	5.94%	0.602%

Sum of corrected areas: 70726326

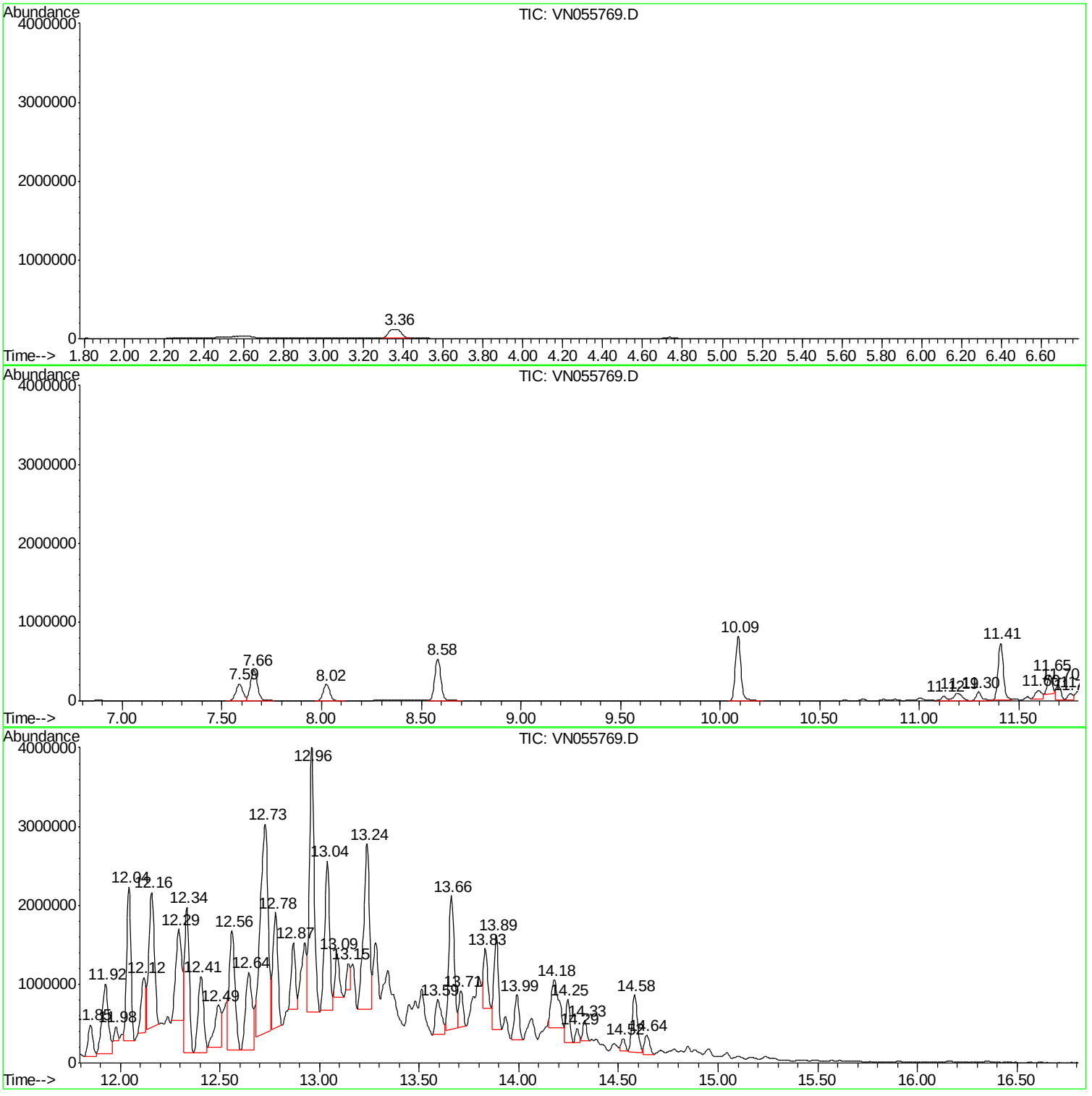
LSC Report - Integrated Chromatogram

Data Path : Z:\voasrv\HPCHEM1\MSVOA N\Data\VN052319\
Data File : VN055769.D
Acq On : 23 May 2019 21:47
Operator : JC/SP
Sample : K2976-04
Misc : 6.67g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 32 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
EP1-SB-E3-4R(17-20)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N052319W.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\VN052319\
Data File : VN055769.D
Acq On : 23 May 2019 21:47
Operator : JC/SP
Sample : K2976-04
Misc : 6.67g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 32 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : EP1-SB-E3-4R(17-20)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N052319W.M
Quant Title : SW846 8260

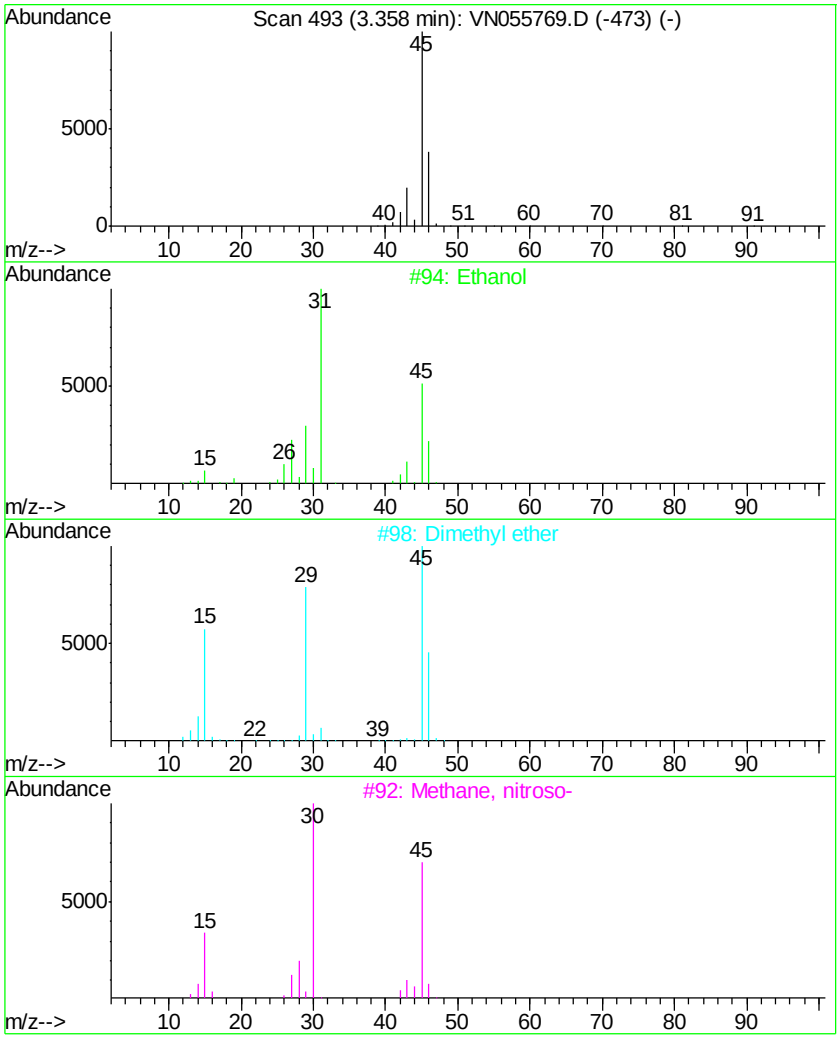
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

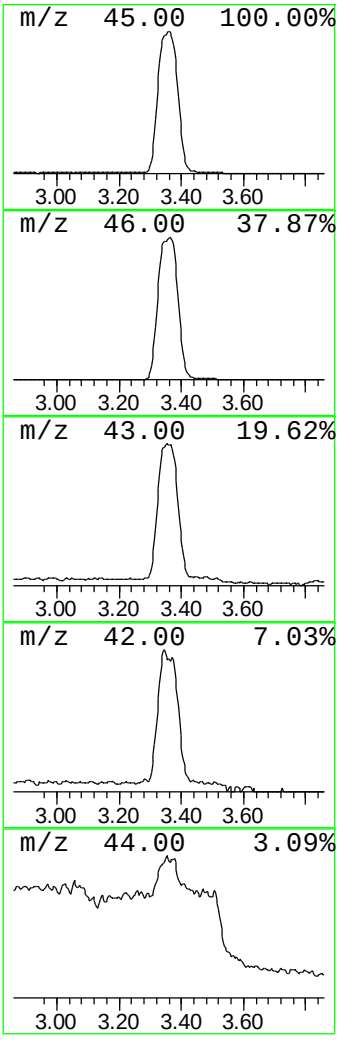
****

Peak Number 1 Ethanol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.36	25.20 ug/l	468718	Pentafluorobenzene	7.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol	46	C2H6O	000064-17-5	64
2	Dimethyl ether	46	C2H6O	000115-10-6	9
3	Methane, nitroso-	45	CH3NO	000865-40-7	4
4	Propanedioic acid, dihydroxy-	136	C3H4O6	000560-27-0	4
5	Formic acid	46	CH2O2	000064-18-6	4





Data Path : Z:\voasrv\HPCHEM1\MSVOA N\Data\VN052319\
Data File : VN055769.D
Acq On : 23 May 2019 21:47
Operator : JC/SP
Sample : K2976-04
Misc : 6.67g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 32 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : EP1-SB-E3-4R(17-20)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N052319W.M
Quant Title : SW846 8260

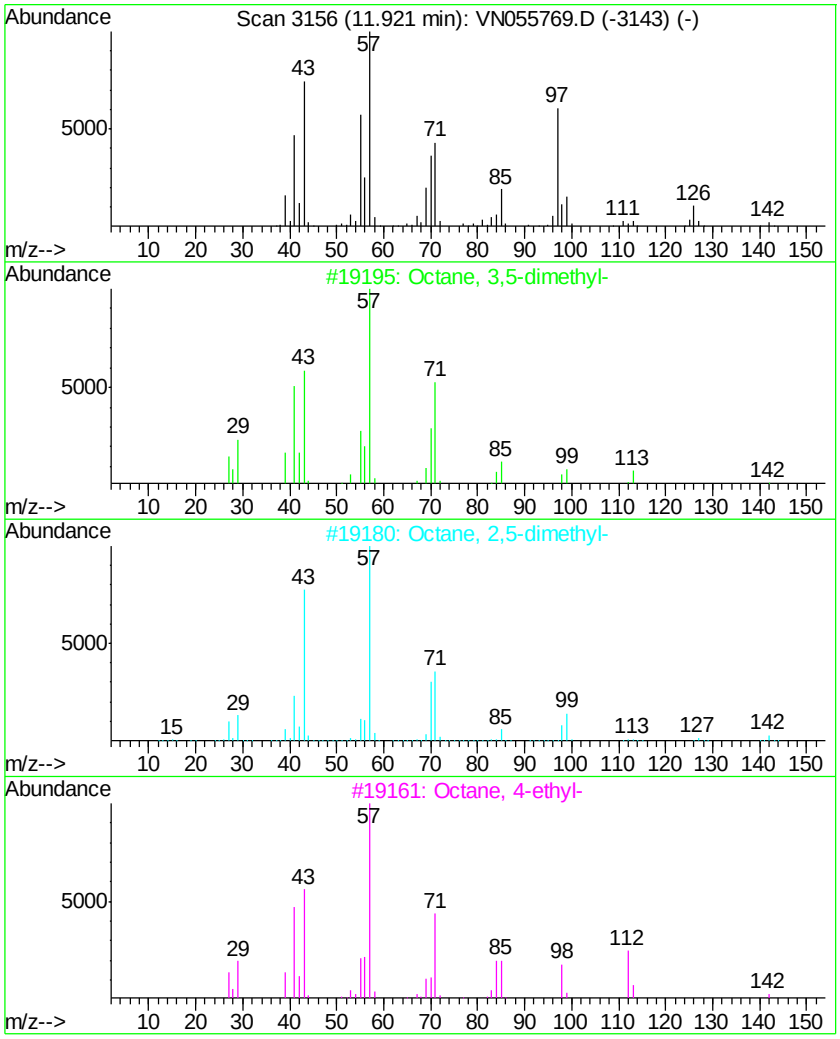
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

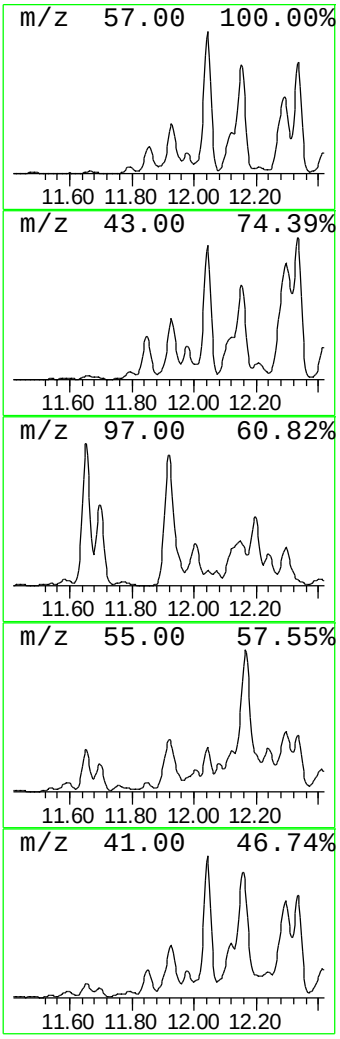
****

Peak Number 2 Octane, 3,5-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	72.85 ug/l	1970150	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	58
2	Octane, 2,5-dimethyl-	142	C10H22	015869-89-3	49
3	Octane, 4-ethyl-	142	C10H22	015869-86-0	47
4	Nonane, 4-methyl-	142	C10H22	017301-94-9	43
5	Heptane, 3-ethyl-2-methyl-	142	C10H22	014676-29-0	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052319\
Data File : VN055769.D
Acq On : 23 May 2019 21:47
Operator : JC/SP
Sample : K2976-04
Misc : 6.67g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 32 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : EP1-SB-E3-4R(17-20)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N052319W.M
Quant Title : SW846 8260

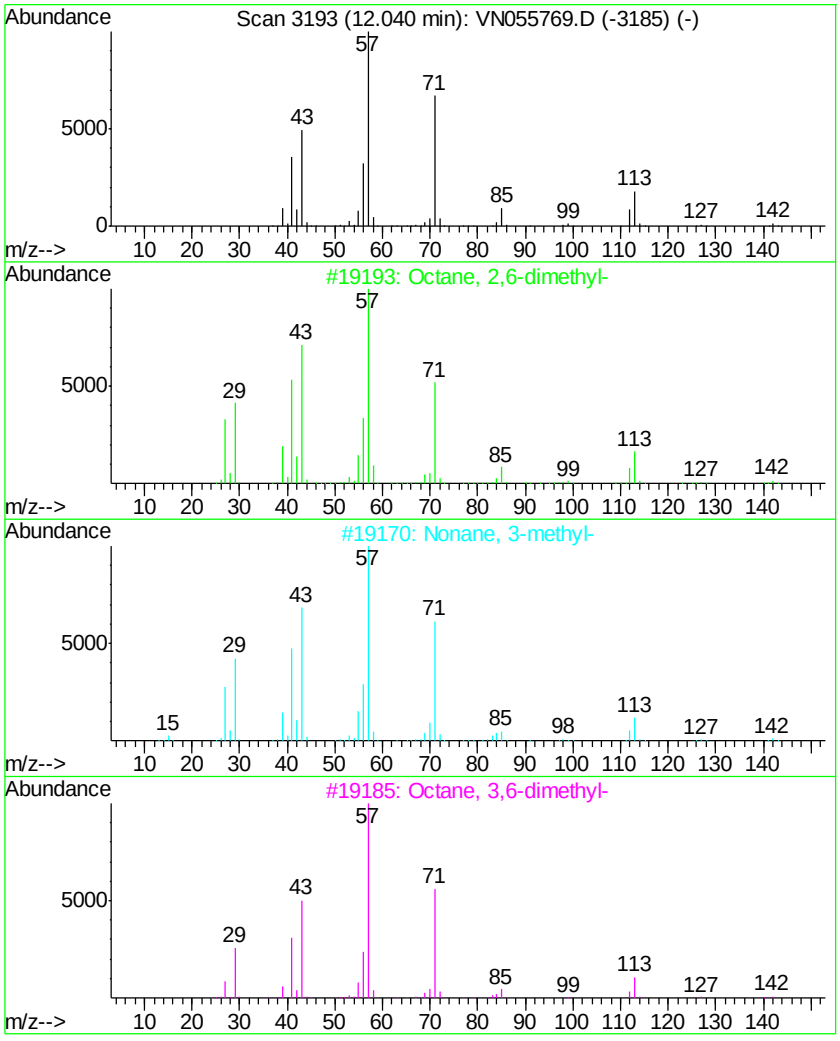
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

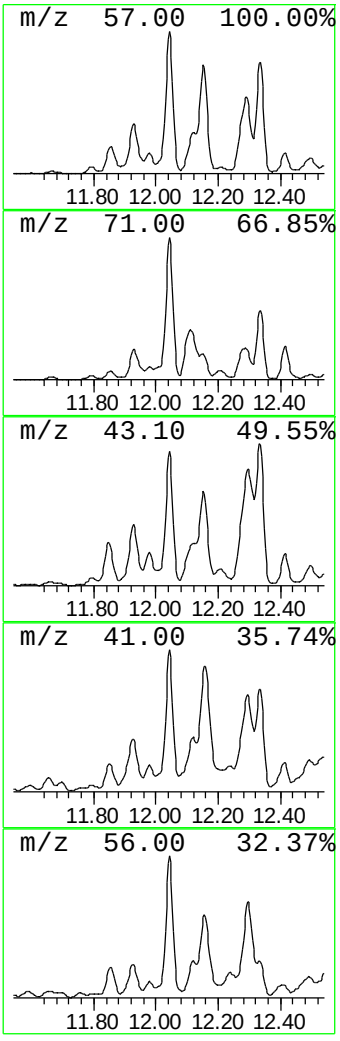
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.04	104.73 ug/l	2832380	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	86
4	Octane, 2,3,7-trimethyl-	156	C11H24	062016-34-6	64
5	Undecane, 6,6-dimethyl-	184	C13H28	017312-76-4	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA N\Data\VN052319\
Data File : VN055769.D
Acq On : 23 May 2019 21:47
Operator : JC/SP
Sample : K2976-04
Misc : 6.67g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 32 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : EP1-SB-E3-4R(17-20)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N052319W.M
Quant Title : SW846 8260

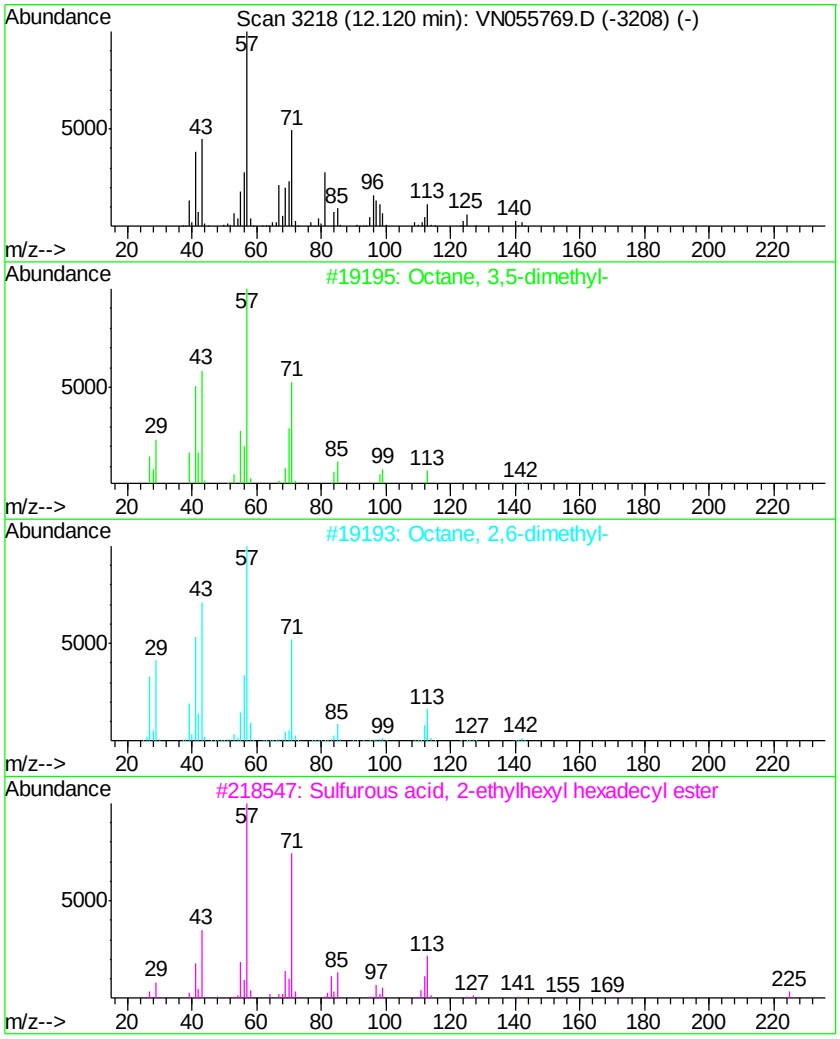
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

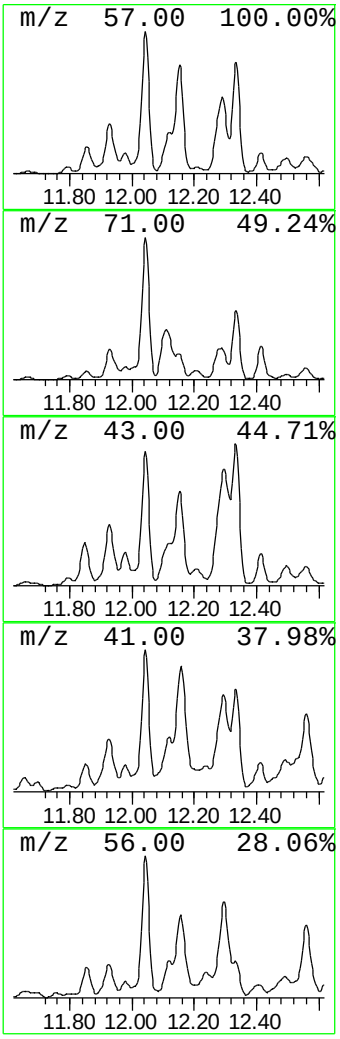
****

Peak Number 4 unknown12.12 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.12	43.05 ug/l	1164220	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	58
2	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	47
3	Sulfurous acid, 2-ethylhexyl hex...	418	C24H50O3S	1000309-19-9	43
4	Nonane, 3-methyl-	142	C10H22	005911-04-6	43
5	Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	43





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052319\
Data File : VN055769.D
Acq On : 23 May 2019 21:47
Operator : JC/SP
Sample : K2976-04
Misc : 6.67g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 32 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : EP1-SB-E3-4R(17-20)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N052319W.M
Quant Title : SW846 8260

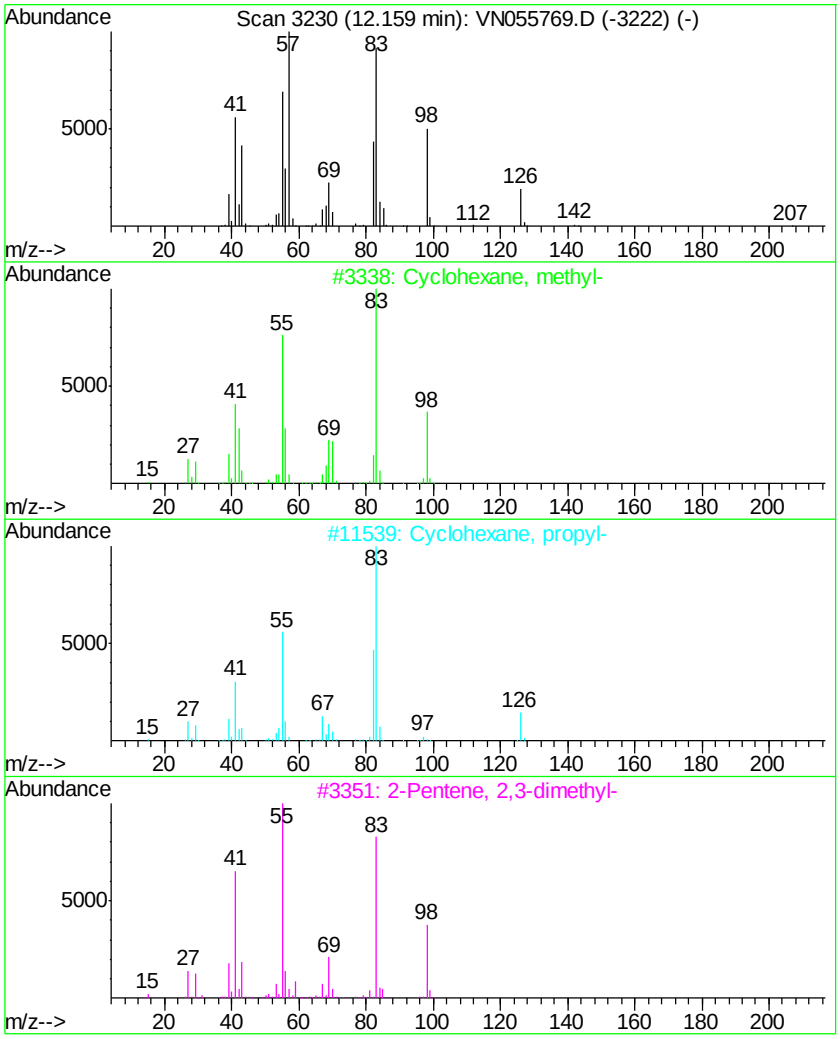
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

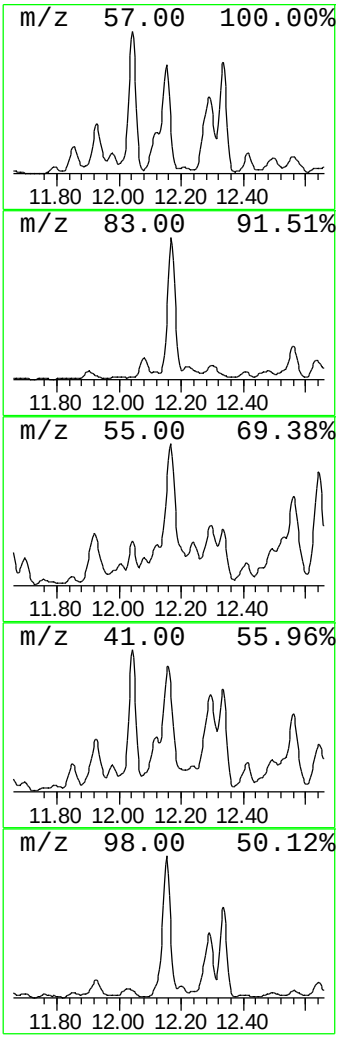
****

Peak Number 5 Cyclohexane, propyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.16	122.31 ug/l	3307860	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, methyl-	98	C7H14	000108-87-2	62
2	Cyclohexane, propyl-	126	C9H18	001678-92-8	53
3	2-Pentene, 2,3-dimethyl-	98	C7H14	010574-37-5	46
4	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	43
5	Cyclopropane, 1,1,2,3-tetramethyl-	98	C7H14	074752-93-5	43





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052319\
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Misc : 6.67g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 32 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : EP1-SB-E3-4R(17-20)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N052319W.M
Quant Title : SW846 8260

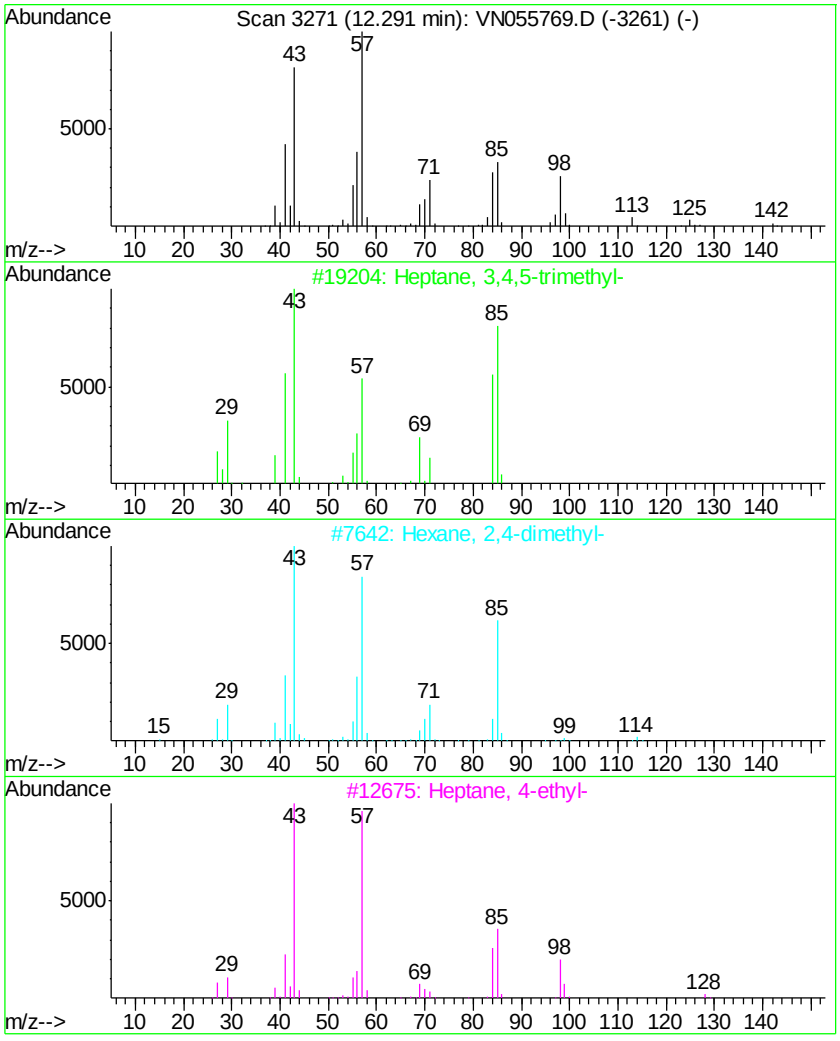
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

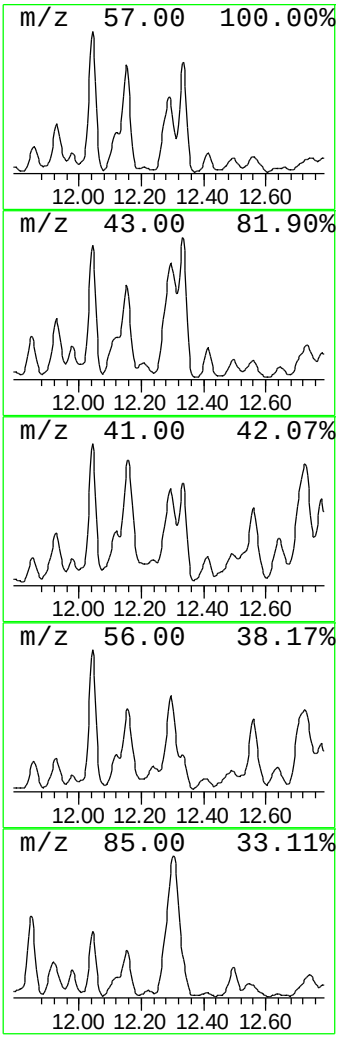
****

Peak Number 6 Heptane, 3,4,5-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.29	91.73 ug/l	2480740	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane, 3,4,5-trimethyl-	142	C10H22	020278-89-1	64
2	Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	58
3	Heptane, 4-ethyl-	128	C9H20	002216-32-2	49
4	Oxalic acid, butyl isohexyl ester	230	C12H22O4	1000309-32-7	47
5	Hexyl isobutyl carbonate	202	C11H22O3	959067-98-2	47





Library Search Compound Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052319\
Data File : VN055769.D
Acq On : 23 May 2019 21:47
Operator : JC/SP
Sample : K2976-04
Misc : 6.67g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 32 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : EP1-SB-E3-4R(17-20)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N052319W.M
Quant Title : SW846 8260

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

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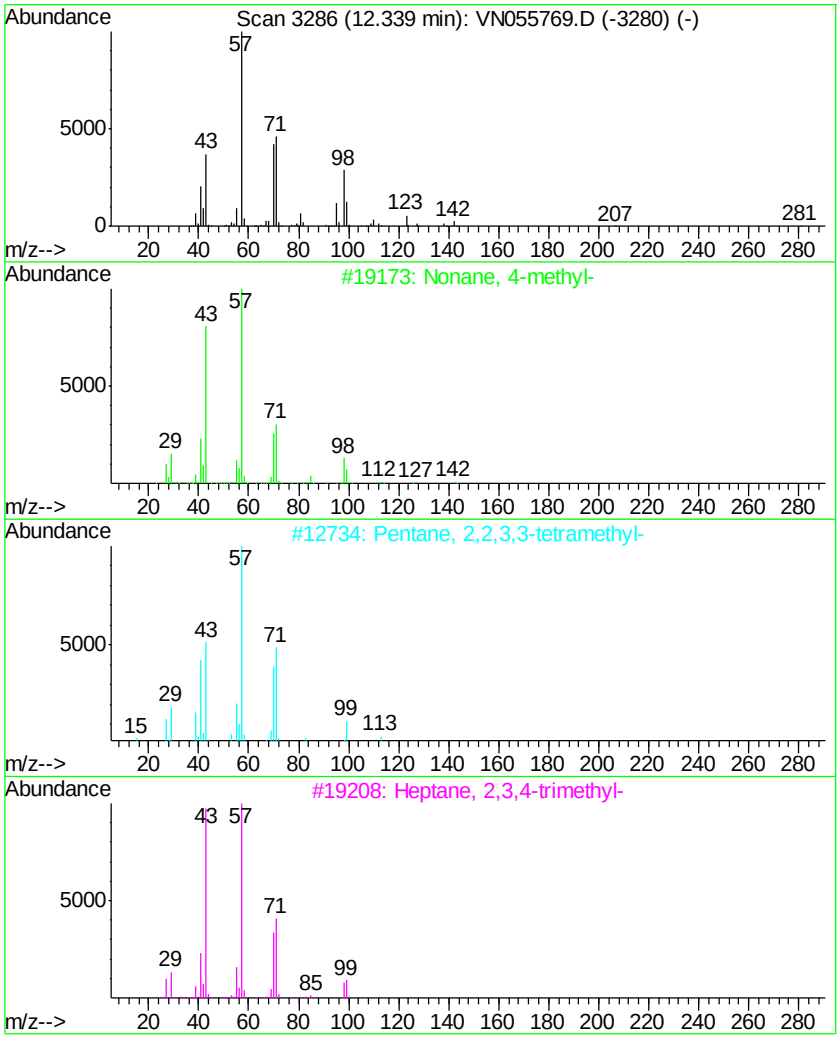
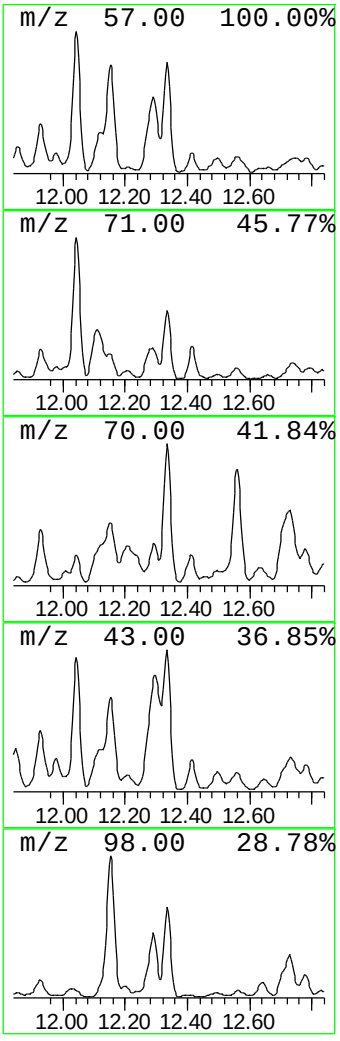
Peak Number 7 Nonane, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.34	101.76 ug/l	2751950	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonane, 4-methyl-	142	C10H22	017301-94-9	72
2	Pentane, 2,2,3,3-tetramethyl-	128	C9H20	007154-79-2	59
3	Heptane, 2,3,4-trimethyl-	142	C10H22	052896-95-4	50
4	Octane, 2,5-dimethyl-	142	C10H22	015869-89-3	42
5	Heptane, 4-propyl-	142	C10H22	003178-29-8	35





Library Search Compound Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA N\Data\VN052319\
Data File : VN055769.D
Acq On : 23 May 2019 21:47
Operator : JC/SP
Sample : K2976-04
Misc : 6.67g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 32 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : EP1-SB-E3-4R(17-20)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N052319W.M
Quant Title : SW846 8260

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

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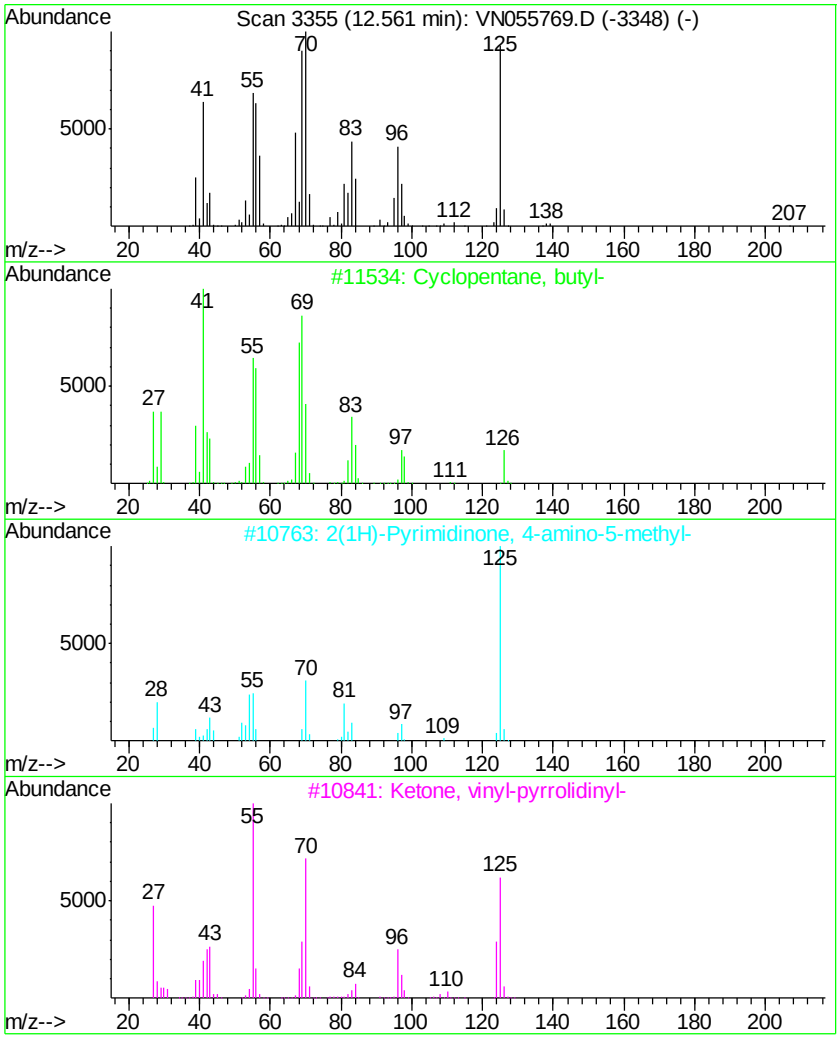
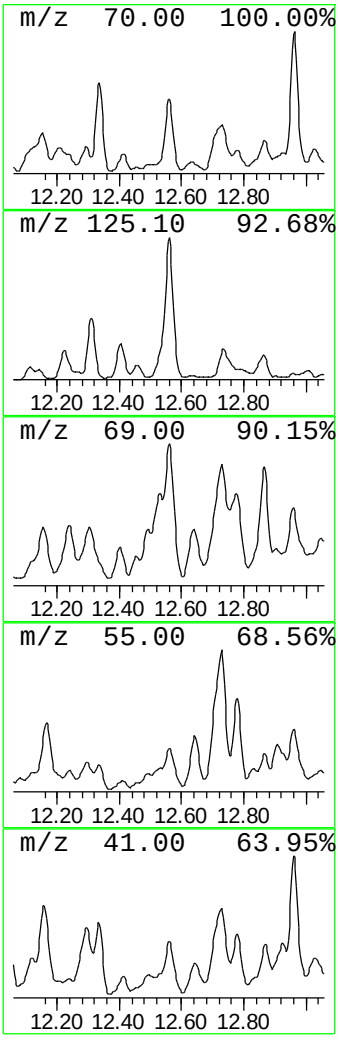
Peak Number 8 Cyclopentane, butyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.56	34.30 ug/l	2954550	1,4-Dichlorobenzene-d4	13.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, butyl-	126	C9H18	002040-95-1	46
2	2(1H)-Pyrimidinone, 4-amino-5-me...	125	C5H7N3O	000554-01-8	43
3	Ketone, vinyl-pyrrolidinyl-	125	C7H11NO	042104-70-1	43
4	1-Nonanol	144	C9H20O	000143-08-8	35
5	cis-1-Butyl-2-methylcyclopropane	112	C8H16	038851-69-3	30





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Data File : VN055769.D
Acq On : 23 May 2019 21:47
Operator : JC/SP
Sample : K2976-04
Misc : 6.67g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 32 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : EP1-SB-E3-4R(17-20)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N052319W.M
Quant Title : SW846 8260

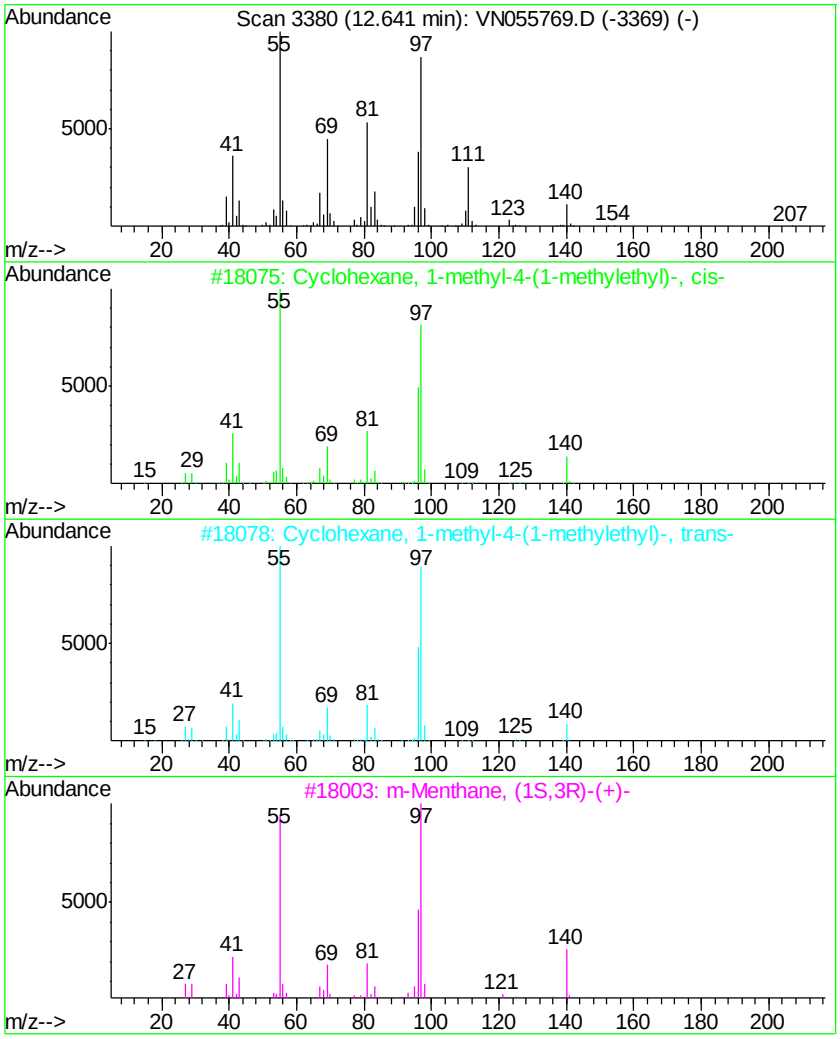
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

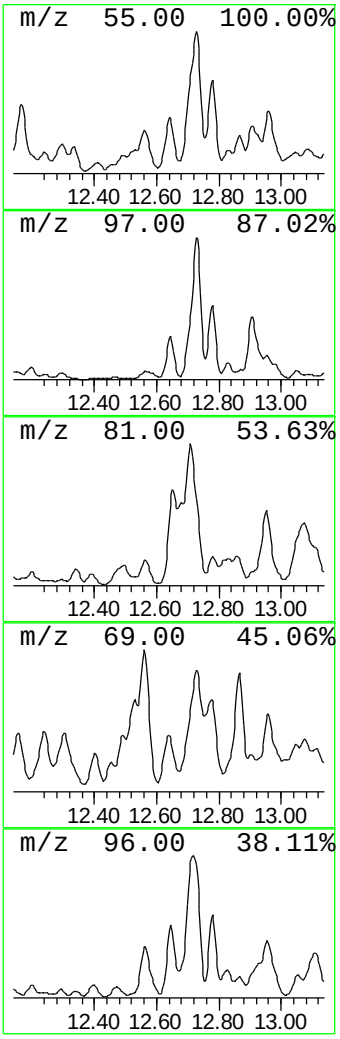
****

Peak Number 9 Cyclohexane, 1-methyl-4-(1-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.64	25.94 ug/l	2234780	1,4-Dichlorobenzene-d4	13.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1-methyl-4-(1-methy...	140	C10H20	006069-98-3	81
2	Cyclohexane, 1-methyl-4-(1-methy...	140	C10H20	001678-82-6	72
3	m-Menthane, (1S,3R)-(+)-	140	C10H20	013837-66-6	72
4	Cyclohexane, 1-methyl-3-(1-methy...	140	C10H20	016580-24-8	59
5	Cyclohexane, 1-methyl-3-propyl-	140	C10H20	004291-80-9	52





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052319\
Data File : VN055769.D
Acq On : 23 May 2019 21:47
Operator : JC/SP
Sample : K2976-04
Misc : 6.67g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 32 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : EP1-SB-E3-4R(17-20)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N052319W.M
Quant Title : SW846 8260

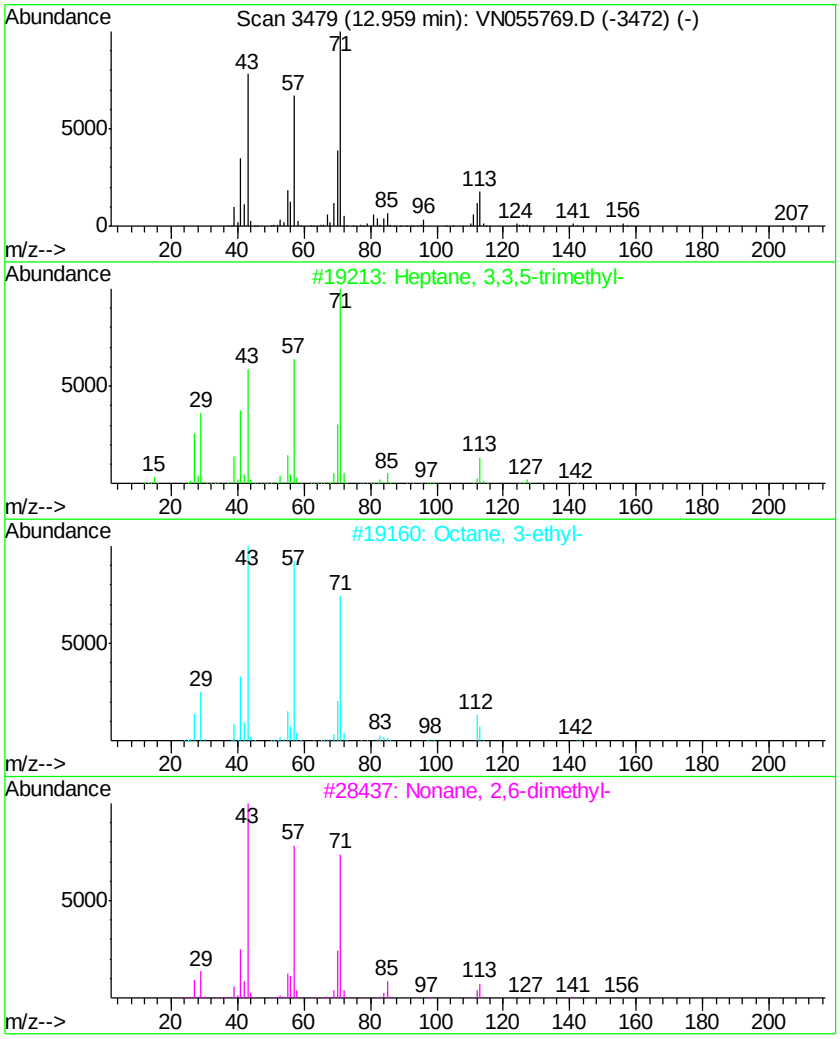
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

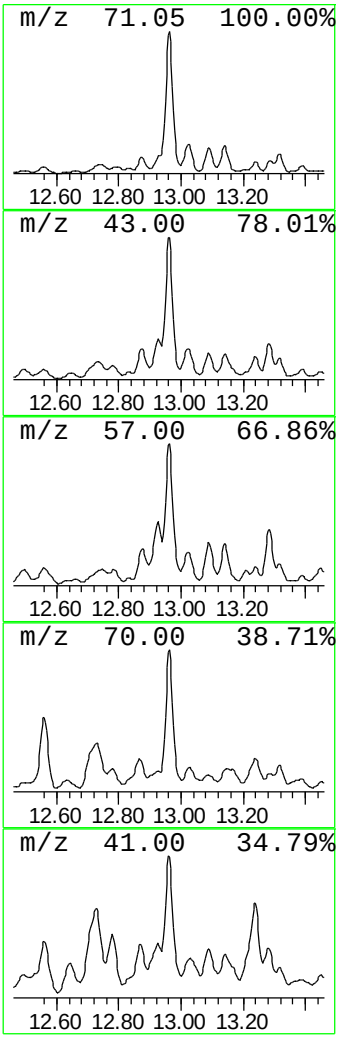
****

Peak Number 10 Heptane, 3,3,5-trimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.96	64.90 ug/l	5590150	1,4-Dichlorobenzene-d4	13.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane, 3,3,5-trimethyl-	142	C10H22	007154-80-5	72
2	Octane, 3-ethyl-	142	C10H22	005881-17-4	72
3	Nonane, 2,6-dimethyl-	156	C11H24	017302-28-2	64
4	4-Methyl-3-heptanol, trifluoroac...	226	C10H17F3O2	1000365-51-8	64
5	2,2'-Bifuran, octahydro-	142	C8H14O2	001592-33-2	59





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052319\
Data File : VN055769.D
Acq On : 23 May 2019 21:47
Operator : JC/SP
Sample : K2976-04
Misc : 6.67g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 32 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : EP1-SB-E3-4R(17-20)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N052319W.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
Ethanol	3.36	25.2	ug/l	468718	1	7.66	929953	50.0
Octane, 3,5-dimet...	11.92	72.8	ug/l	1970150	3	11.41	1352210	50.0
Octane, 2,6-dimet...	12.04	104.7	ug/l	2832380	3	11.41	1352210	50.0
unknown12.12	12.12	43.0	ug/l	1164220	3	11.41	1352210	50.0
Cyclohexane, propyl-	12.16	122.3	ug/l	3307860	3	11.41	1352210	50.0
Heptane, 3,4,5-tr...	12.29	91.7	ug/l	2480740	3	11.41	1352210	50.0
Nonane, 4-methyl-	12.34	101.8	ug/l	2751950	3	11.41	1352210	50.0
Cyclopentane, butyl-	12.56	34.3	ug/l	2954550	4	13.34	4307030	50.0
Cyclohexane, 1-me...	12.64	25.9	ug/l	2234780	4	13.34	4307030	50.0
Heptane, 3,3,5-tr...	12.96	64.9	ug/l	5590150	4	13.34	4307030	50.0