LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN032319\
Data File : VN054631.D
Acq On : 24 Mar 2019 4:20
Operator : JC/SP
Sample : K2043-12
Misc : 6.52g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 39 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : WP022SB443-190319-(16-18)

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\82N032019W.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	2.510	203	229	230	rBV4	42568	117862	2.09%	0.223%
2	2.558	231	244	258	rVB2	130355	270800	4.80%	0.513%
3	7.590	1787	1809	1819	rBV	362992	900879	15.96%	1.706%
4	7.661	1819	1831	1852	rVB	641149	1549892	27.46%	2.936%
5	8.027	1927	1945	1967	rBV3	501611	1235809	21.89%	2.341%
6	8.583	2103	2118	2150	rVB	980270	2115238	37.47%	4.007%
7	9.654	2438	2451	2462	rBV6	26048	61353	1.09%	0.116%
8	9.866	2498	2517	2530	rBV7	24672	73388	1.30%	0.139%
9	10.088	2573	2586	2627	rVV	1490309	3000583	53.16%	5.684%
10	10.718	2769	2782	2792	rVV2	45862	83249	1.47%	0.158%
11	10.818	2803	2813	2826	rBV3	41193	90471	1.60%	0.171%
12	10.950	2847	2854	2861	rVV3	37345	60015	1.06%	0.114%
13	11.001	2861	2870	2882	rVB2	97612	179790	3.19%	0.341%
14	11.123	2895	2908	2914	rBV5	63861	126136	2.23%	0.239%
15	11.297	2949	2962	2980	rBV	205778	397158	7.04%	0.752%
16	11.432	2983	3004	3031	rBV2	1890336	5644479	100.00%	10.691%
17	11.541	3033	3038	3044	rVB4	48541	57806	1.02%	0.109%
18	11.596	3045	3055	3063	rBV6	110739	217143	3.85%	0.411%
19	11.654	3064	3073	3081	rBV3	230424	430901	7.63%	0.816%
20	11.757	3096	3105	3110	rBV3	76161	129094	2.29%	0.245%
21	11.853	3127	3135	3142	rBV2	181792	280620	4.97%	0.532%
22	11.924	3143	3157	3169	rBV6	506077	1262746	22.37%	2.392%
23	11.979	3170	3174	3178	rBV2	73516	78551	1.39%	0.149%
24	12.043	3187	3194	3202	rVB	734492	1041775	18.46%	1.973%
25	12.117	3208	3217	3222	rBV2	449718	789326	13.98%	1.495%
26	12.156	3223	3229	3240	rVB4	844064	1535414	27.20%	2.908%
27	12.291	3260	3271	3281	rVB6	626991	1363519	24.16%	2.583%
28	12.403	3294	3306	3317	rBV2	1247673	2374508	42.07%	4.498%
29	12.561	3347	3355	3369	rVB3	1012705	1977428	35.03%	3.746%
30	12.644	3369	3381	3391	rBV7	487821	1226610	21.73%	2.323%
31	12.728	3393	3407	3416	rVV6	1194172	3221714	57.08%	6.102%
32	12.779	3419	3423	3434	rVB5	660405	975838	17.29%	1.848%
33	12.869	3444	3451	3457	rBV5	412356	595789	10.56%	1.129%
34	12.959	3474	3479	3493	rVB7	538601	1028140	18.21%	1.947%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN032319\
Data File : VN054631.D
Acq On : 24 Mar 2019 4:20
Operator : JC/SP
Sample : K2043-12
Misc : 6.52g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 39 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : WP022SB443-190319-(16-18)

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\82N032019W.M
Title : SW846 8260

35	13.088	3514	3519	3530	rVB4	324486	450561	7.98%	0.853%
36	13.239	3552	3566	3574	rBV3	1439656	2953596	52.33%	5.595%
37	13.342	3590	3598	3624	rVB	1250685	2706905	47.96%	5.127%
38	13.660	3688	3697	3707	rBV3	1705406	2931164	51.93%	5.552%
39	13.992	3792	3800	3809	rBV5	331075	605558	10.73%	1.147%
40	14.178	3847	3858	3884	rVB7	1211014	3751271	66.46%	7.105%
41	14.297	3886	3895	3900	rBV3	506364	880672	15.60%	1.668%
42	14.332	3901	3906	3913	rVB	525882	677918	12.01%	1.284%
43	14.583	3975	3984	3996	rBV4	470603	998012	17.68%	1.890%
44	14.647	3997	4004	4013	rVB2	288287	441935	7.83%	0.837%
45	14.850	4062	4067	4074	rVB3	219934	256286	4.54%	0.485%
46	15.043	4121	4127	4136	rVB5	209376	357073	6.33%	0.676%
47	16.606	4603	4613	4625	rBV	657826	1289325	22.84%	2.442%

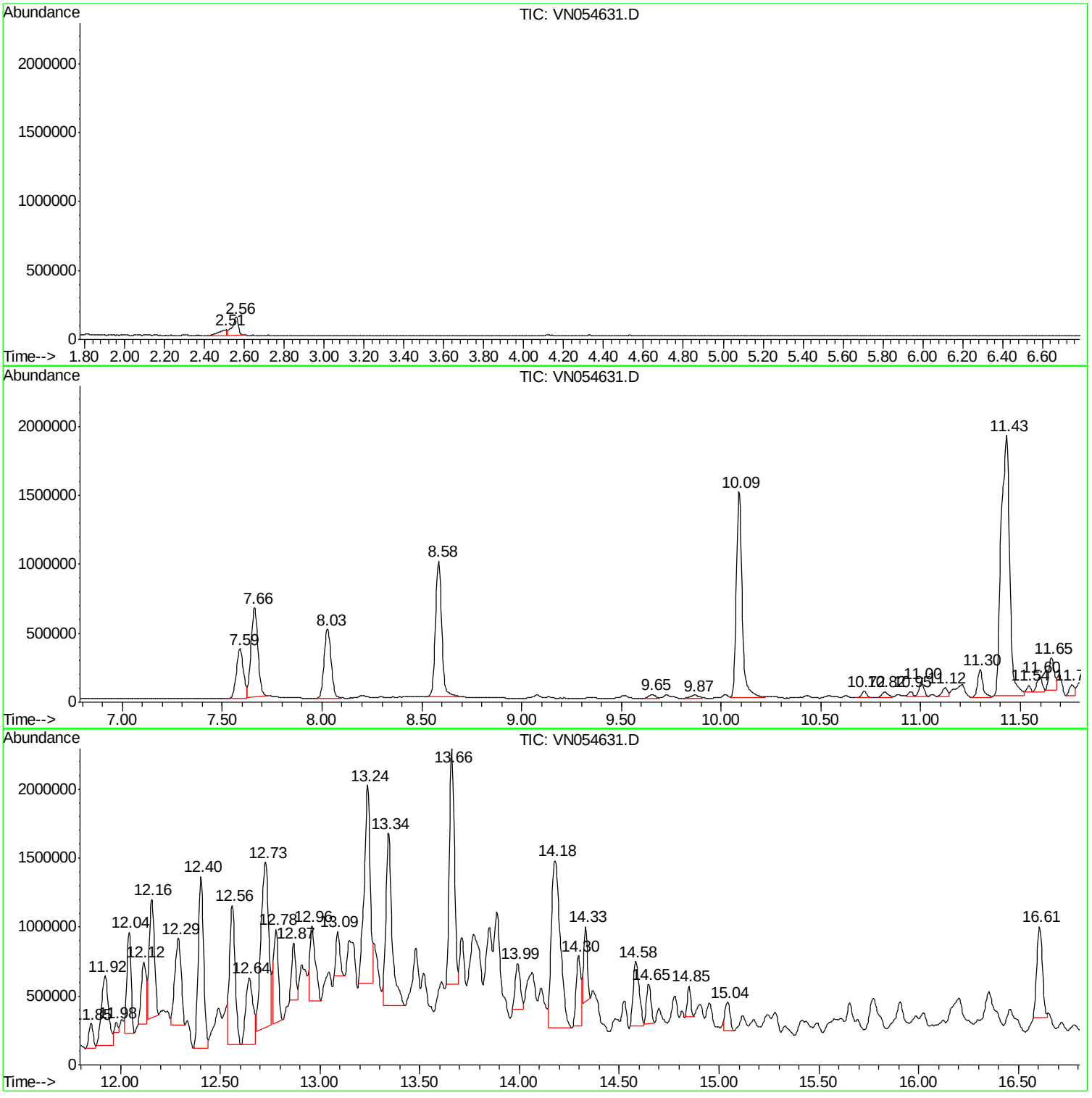
Sum of corrected areas: 52794300

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN032319\
Data File : VN054631.D
Acq On : 24 Mar 2019 4:20
Operator : JC/SP
Sample : K2043-12
Misc : 6.52g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 39 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WP022SB443-190319-(16-18)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N032019W.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\VN032319\
Data File : VN054631.D
Acq On : 24 Mar 2019 4:20
Operator : JC/SP
Sample : K2043-12
Misc : 6.52g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 39 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : WP022SB443-190319-(16-18)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N032019W.M
Quant Title : SW846 8260

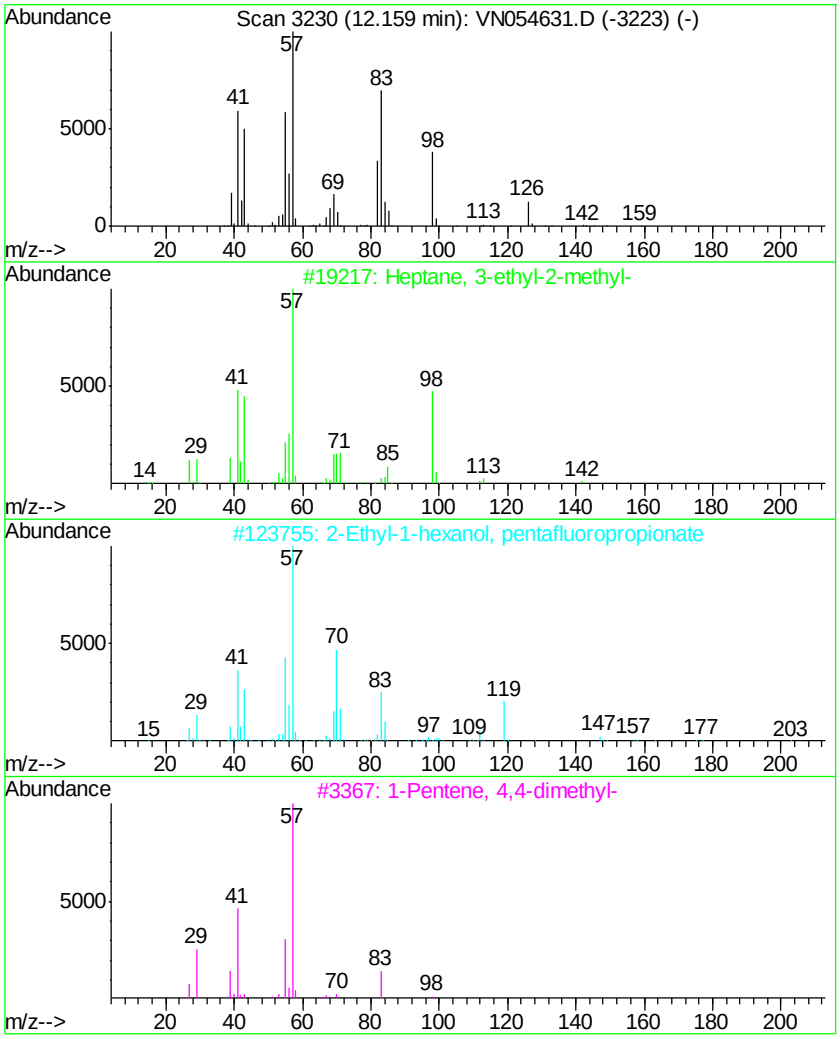
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

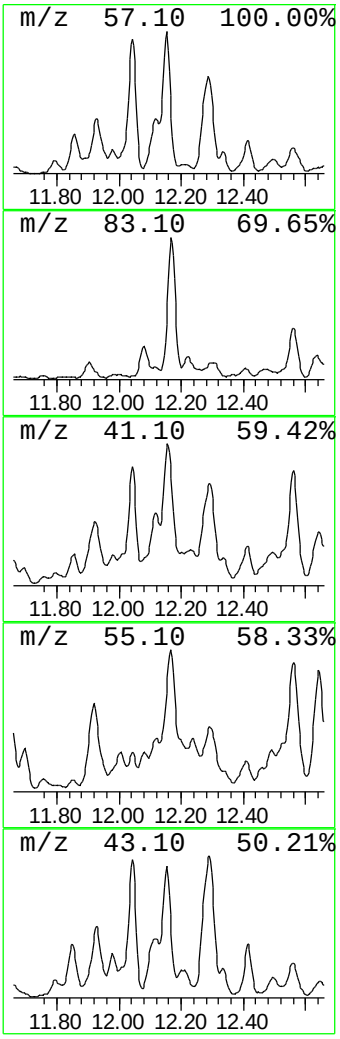
****

Peak Number 1 unknown12.16 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.16	13.60 ug/l	1535410	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane, 3-ethyl-2-methyl-	142	C10H22	014676-29-0	43
2	2-Ethyl-1-hexanol, pentafluoropr...	276	C11H17F5O2	1000365-51-1	43
3	1-Pentene, 4,4-dimethyl-	98	C7H14	000762-62-9	38
4	Heptane, 4-(1-methylethyl)-	142	C10H22	052896-87-4	35
5	2-Ethyl-1-hexanol, trifluoroacetate	226	C10H17F3O2	1000365-19-6	35





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN032319\
Data File : VN054631.D
Acq On : 24 Mar 2019 4:20
Operator : JC/SP
Sample : K2043-12
Misc : 6.52g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 39 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : WP022SB443-190319-(16-18)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N032019W.M
Quant Title : SW846 8260

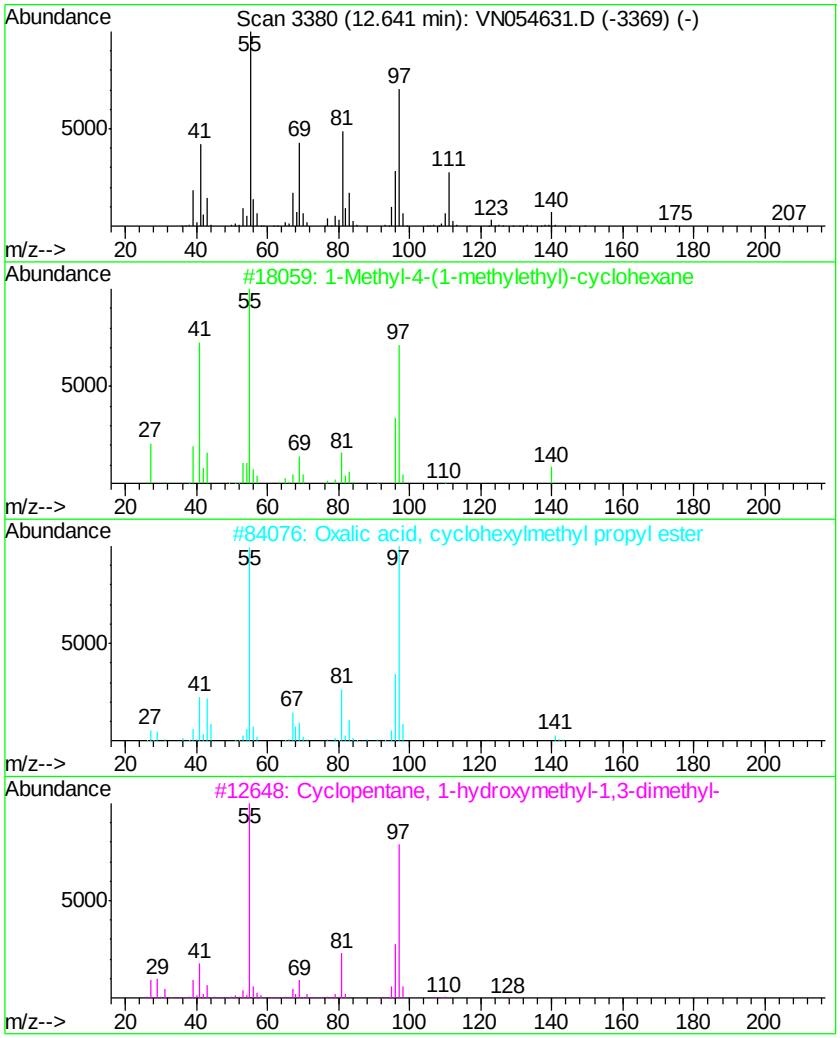
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

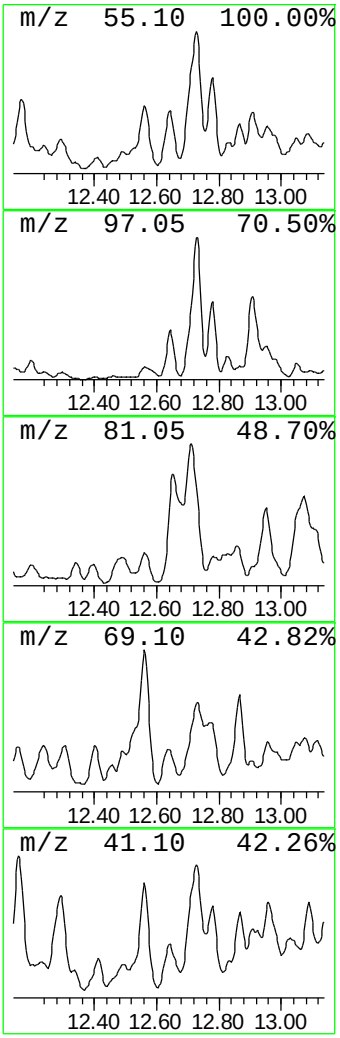
****

Peak Number 2 1-Methyl-4-(1-methylethyl)-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.64	22.66 ug/l	1226610	1,4-Dichlorobenzene-d4	13.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Methyl-4-(1-methylethyl)-cyclo...	140	C10H20	000099-82-1	64
2	Oxalic acid, cyclohexylmethyl pr...	228	C12H20O4	1000309-68-1	59
3	Cyclopentane, 1-hydroxymethyl-1,...	128	C8H16O	1000156-73-8	59
4	Cyclohexane, 1-methyl-3-propyl-	140	C10H20	004291-80-9	58
5	Cyclopentane, 1-methyl-3-(2-meth...	140	C10H20	029053-04-1	58





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN032319\
Data File : VN054631.D
Acq On : 24 Mar 2019 4:20
Operator : JC/SP
Sample : K2043-12
Misc : 6.52g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 39 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : WP022SB443-190319-(16-18)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N032019W.M
Quant Title : SW846 8260

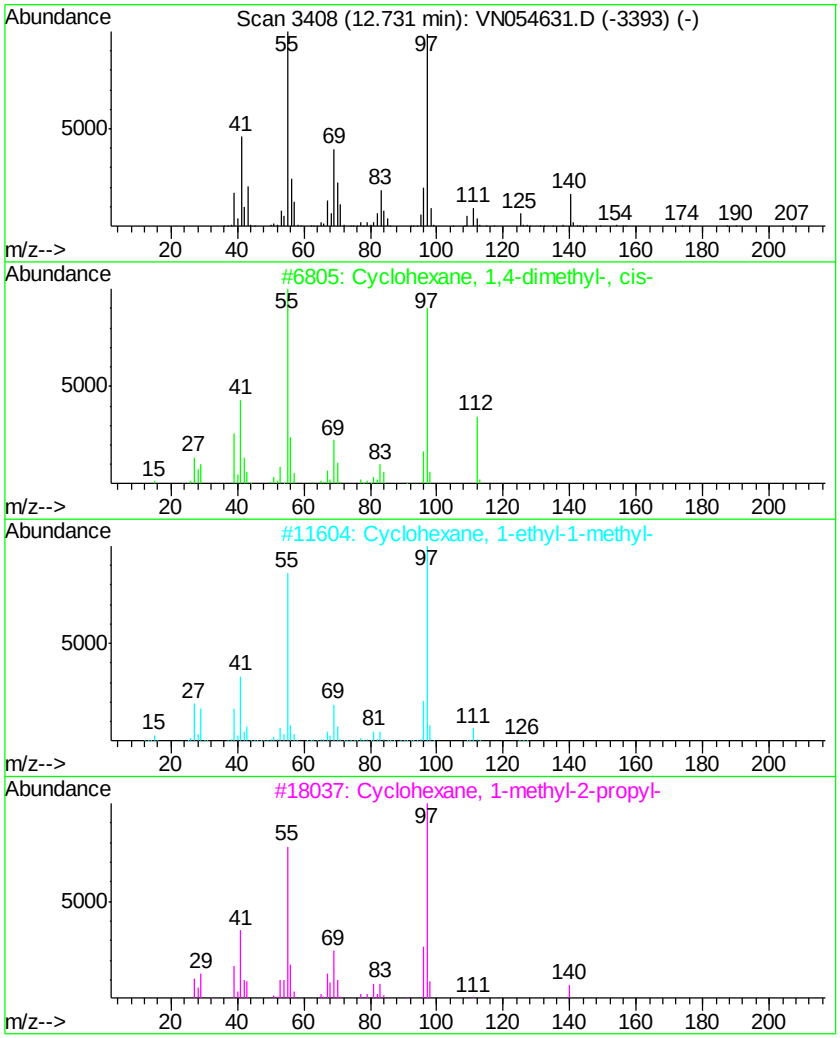
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

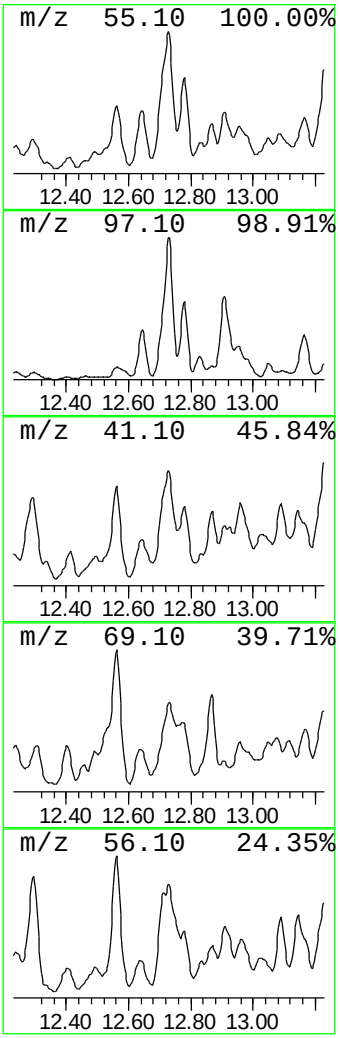
****

Peak Number 3 Cyclohexane, 1,4-dimethyl-,... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.73	59.51 ug/l	3221710	1,4-Dichlorobenzene-d4	13.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,4-dimethyl-, cis-	112	C8H16	000624-29-3	80
2	Cyclohexane, 1-ethyl-1-methyl-	126	C9H18	004926-90-3	58
3	Cyclohexane, 1-methyl-2-propyl-	140	C10H20	004291-79-6	58
4	Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	50
5	Cyclohexane, 1-methyl-4-(1-methy...	140	C10H20	006069-98-3	46





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN032319\
Data File : VN054631.D
Acq On : 24 Mar 2019 4:20
Operator : JC/SP
Sample : K2043-12
Misc : 6.52g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 39 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : WP022SB443-190319-(16-18)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N032019W.M
Quant Title : SW846 8260

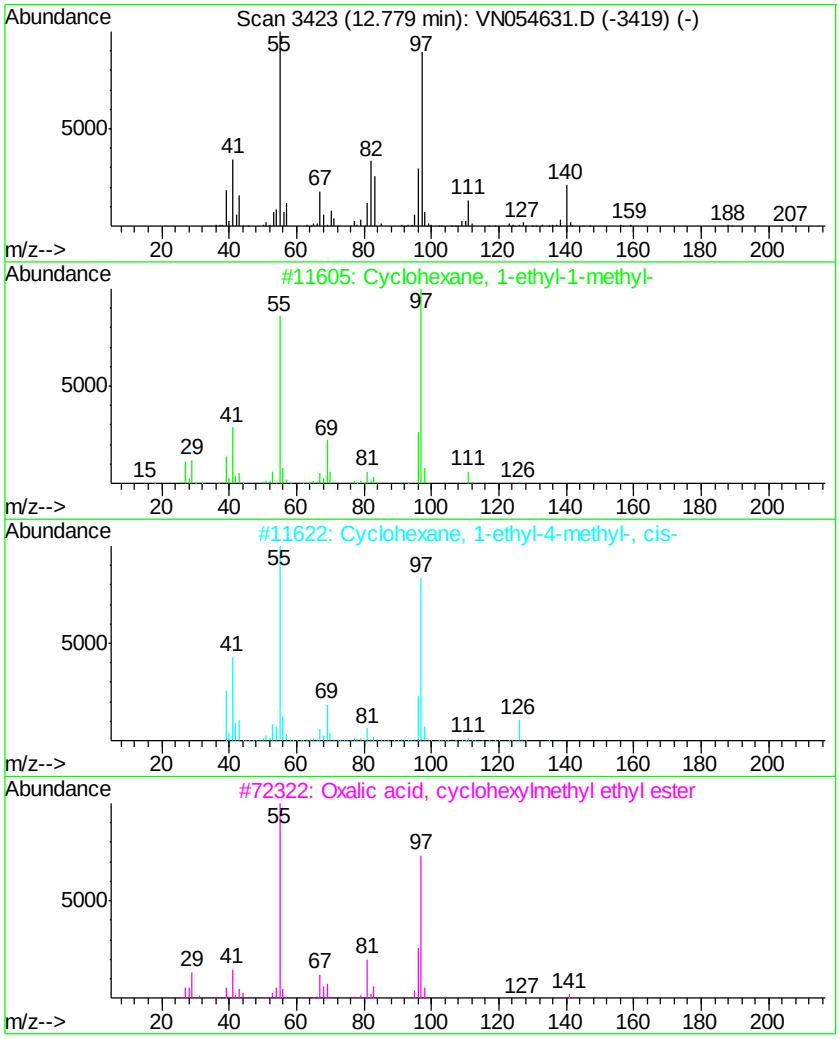
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

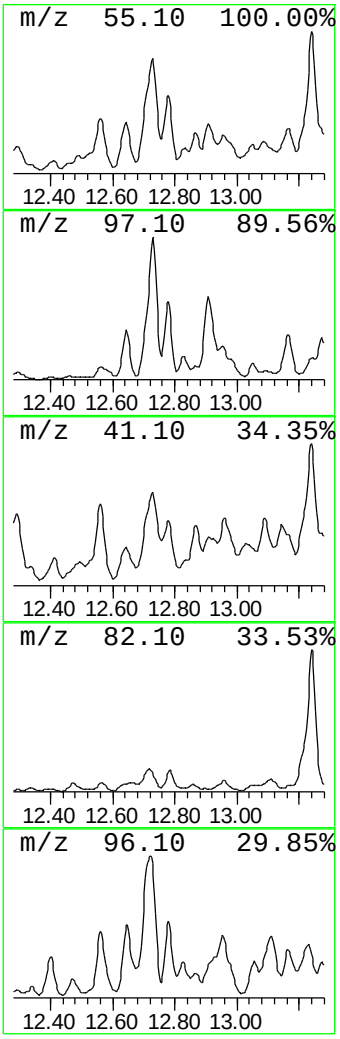
****

Peak Number 4 Cyclohexane, 1-ethyl-1-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.78	18.03 ug/l	975838	1,4-Dichlorobenzene-d4	13.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1-ethyl-1-methyl-	126	C9H18	004926-90-3	58
2	Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	004926-78-7	50
3	Oxalic acid, cyclohexylmethyl et...	214	C11H18O4	1000309-68-0	50
4	Sulfurous acid, di(cyclohexylmet...	274	C14H26O3S	1000309-22-7	50
5	Oxalic acid, cyclohexylmethyl de...	326	C19H34O4	1000309-68-7	50





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN032319\
Data File : VN054631.D
Acq On : 24 Mar 2019 4:20
Operator : JC/SP
Sample : K2043-12
Misc : 6.52g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 39 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : WP022SB443-190319-(16-18)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N032019W.M
Quant Title : SW846 8260

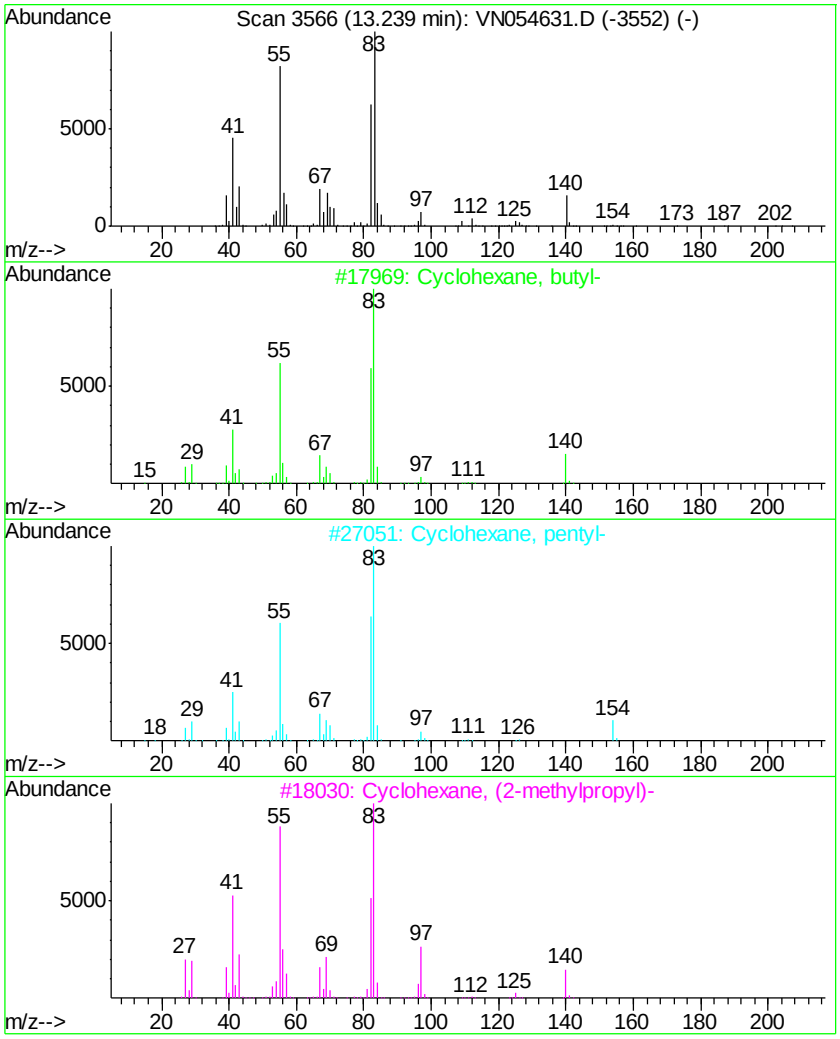
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

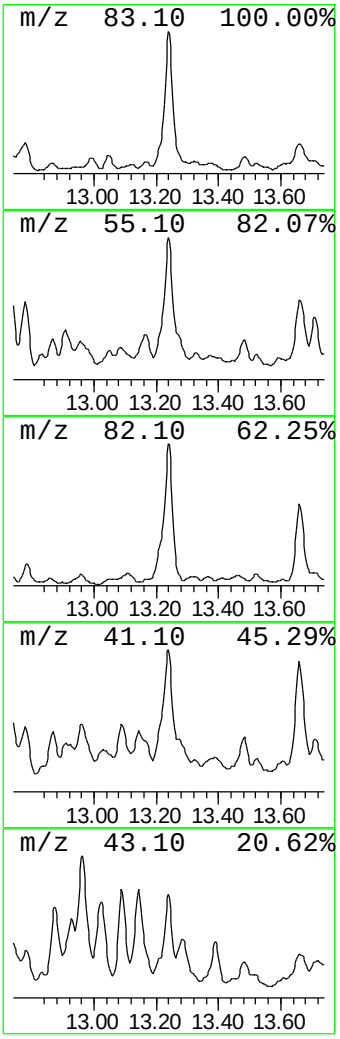
****

Peak Number 5 Cyclohexane, butyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.24	54.56 ug/l	2953600	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	87
3	Cyclohexane, (2-methylpropyl)-	140	C10H20	001678-98-4	83
4	Cyclohexane, (1-methylethyl)-	126	C9H18	000696-29-7	72
5	Cyclohexane, propyl-	126	C9H18	001678-92-8	72





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN032319\
Data File : VN054631.D
Acq On : 24 Mar 2019 4:20
Operator : JC/SP
Sample : K2043-12
Misc : 6.52g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 39 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : WP022SB443-190319-(16-18)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N032019W.M
Quant Title : SW846 8260

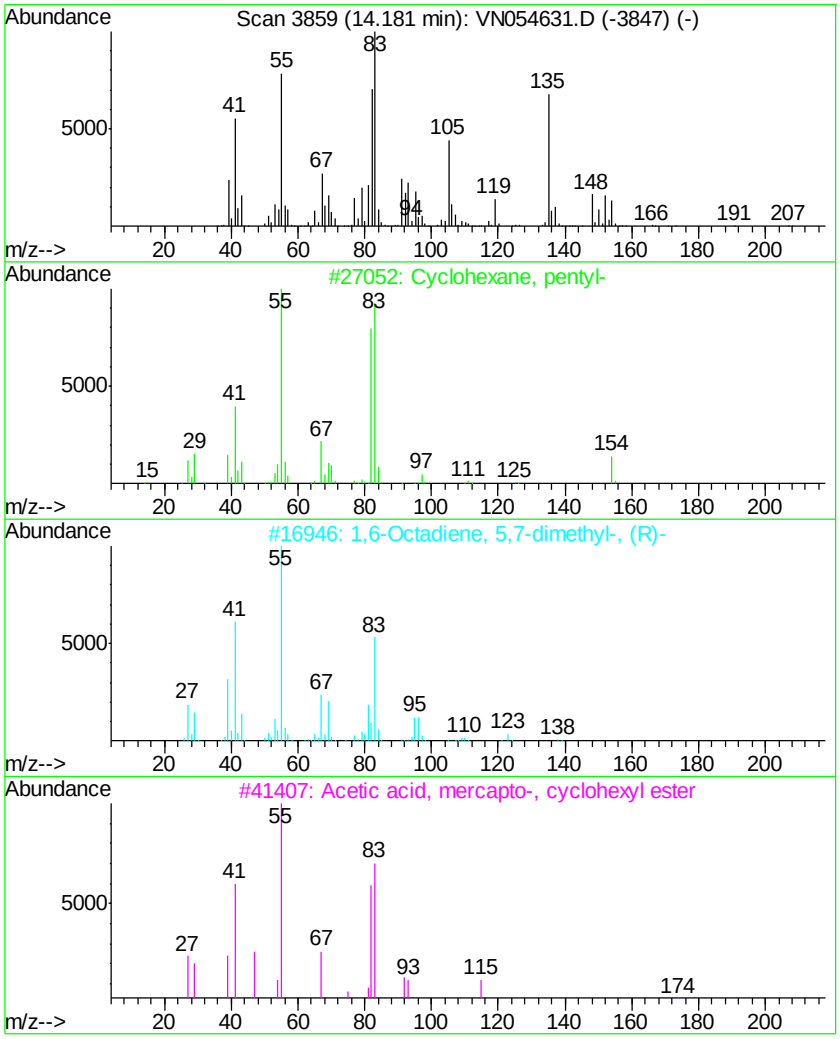
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

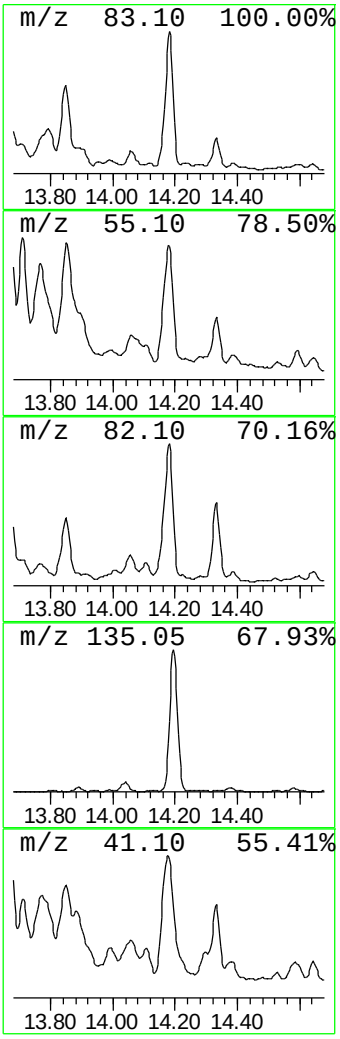
****

Peak Number 6 Cyclohexane, pentyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.18	69.29 ug/l	3751270	1,4-Dichlorobenzene-d4	13.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, pentyl-	154	C11H22	004292-92-6	86
2	1,6-Octadiene, 5,7-dimethyl-, (R)-	138	C10H18	085006-04-8	38
3	Acetic acid, mercapto-, cyclohex...	174	C8H14O2S	016849-98-2	35
4	Cyclohexane, (1-methylethyl)-	126	C9H18	000696-29-7	35
5	Cyclohexane, hexyl-	168	C12H24	004292-75-5	35





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN032319\
Data File : VN054631.D
Acq On : 24 Mar 2019 4:20
Operator : JC/SP
Sample : K2043-12
Misc : 6.52g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 39 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : WP022SB443-190319-(16-18)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N032019W.M
Quant Title : SW846 8260

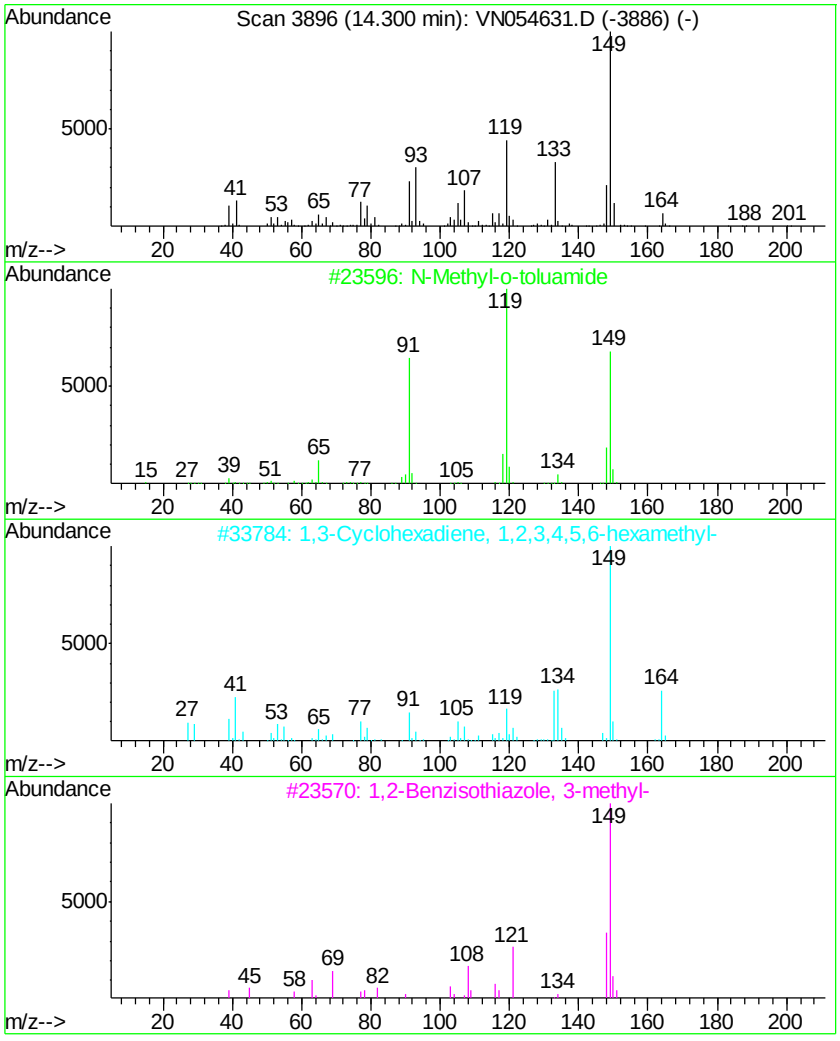
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

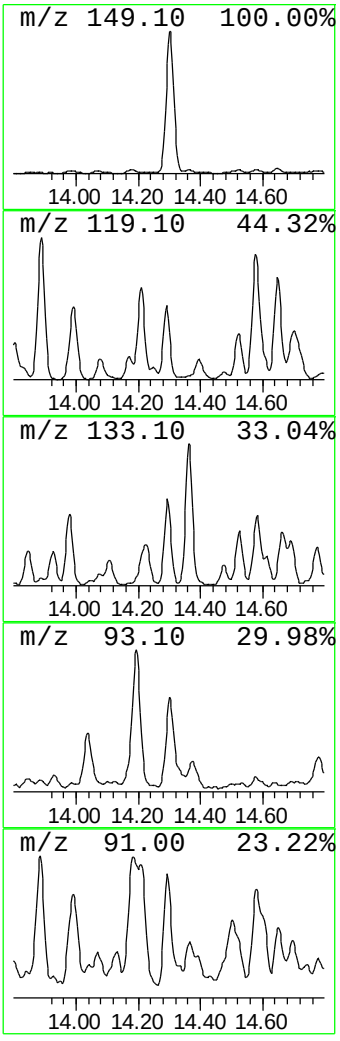
****

Peak Number 7 N-Methyl-o-toluamide Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.30	16.27 ug/l	880672	1,4-Dichlorobenzene-d4	13.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	N-Methyl-o-toluamide	149	C9H11NO	002170-09-4	64
2	1,3-Cyclohexadiene, 1,2,3,4,5,6-...	164	C12H20	1000152-09-6	47
3	1,2-Benzisothiazole, 3-methyl-	149	C8H7NS	006187-89-9	38
4	Benzaldehyde, 3-pentafluoropheno...	332	C15H9F5O3	329222-68-6	35
5	7-Methylthieno[3,2-b]pyridine	149	C8H7NS	013362-83-9	35





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN032319\
Data File : VN054631.D
Acq On : 24 Mar 2019 4:20
Operator : JC/SP
Sample : K2043-12
Misc : 6.52g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 39 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : WP022SB443-190319-(16-18)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N032019W.M
Quant Title : SW846 8260

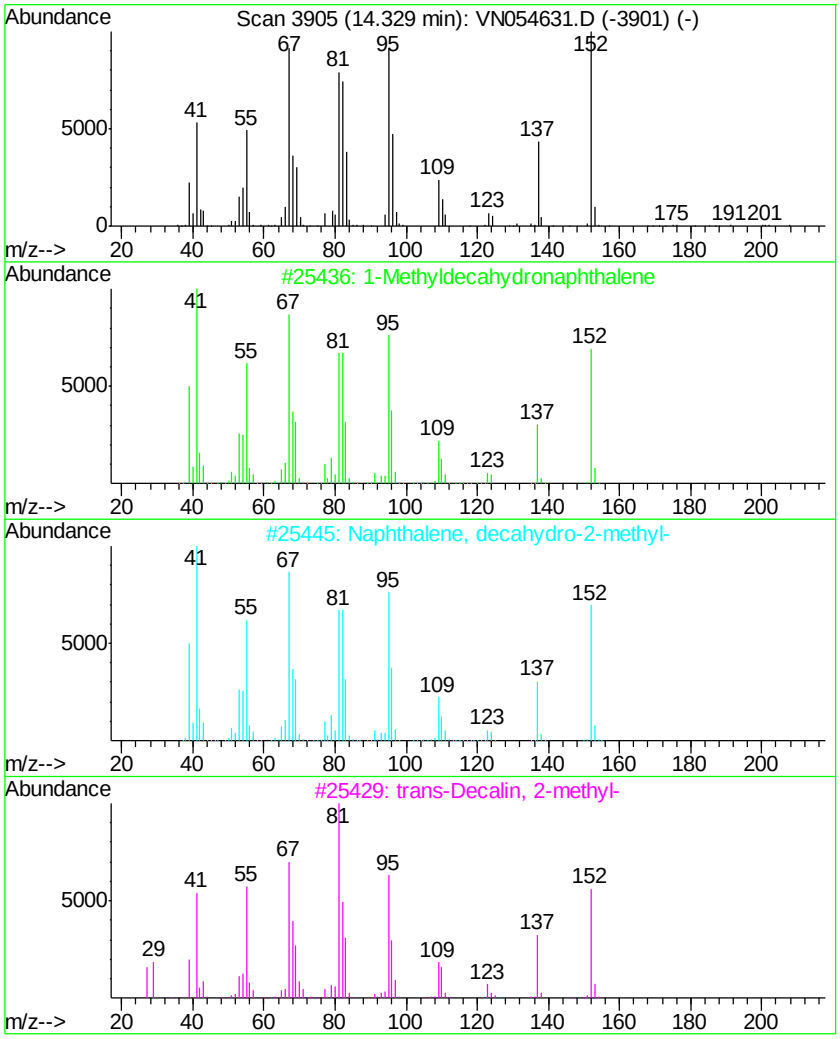
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

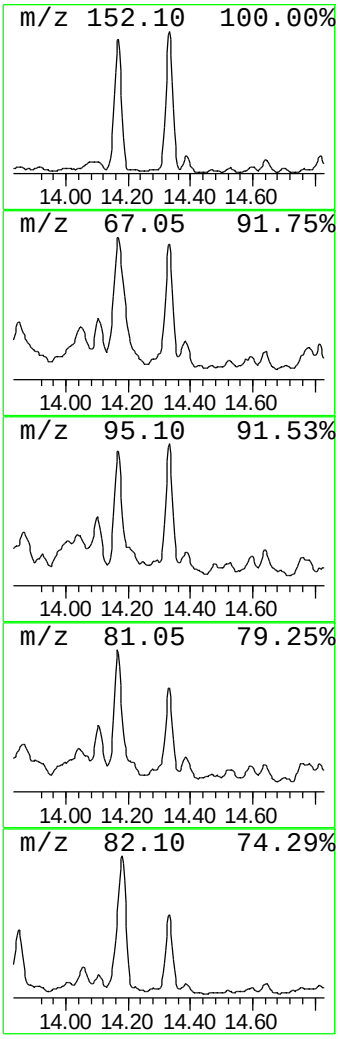
****

Peak Number 8 1-Methyldecahydronaphthalene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.33	12.52 ug/l	677918	1,4-Dichlorobenzene-d4	13.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Methyldecahydronaphthalene	152	C11H20	002958-75-0	94
2	Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	94
3	trans-Decalin, 2-methyl-	152	C11H20	1000152-47-3	90
4	cis-Decalin, 2-syn-methyl-	152	C11H20	1000155-85-6	83
5	Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	64





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN032319\
Data File : VN054631.D
Acq On : 24 Mar 2019 4:20
Operator : JC/SP
Sample : K2043-12
Misc : 6.52g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 39 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : WP022SB443-190319-(16-18)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N032019W.M
Quant Title : SW846 8260

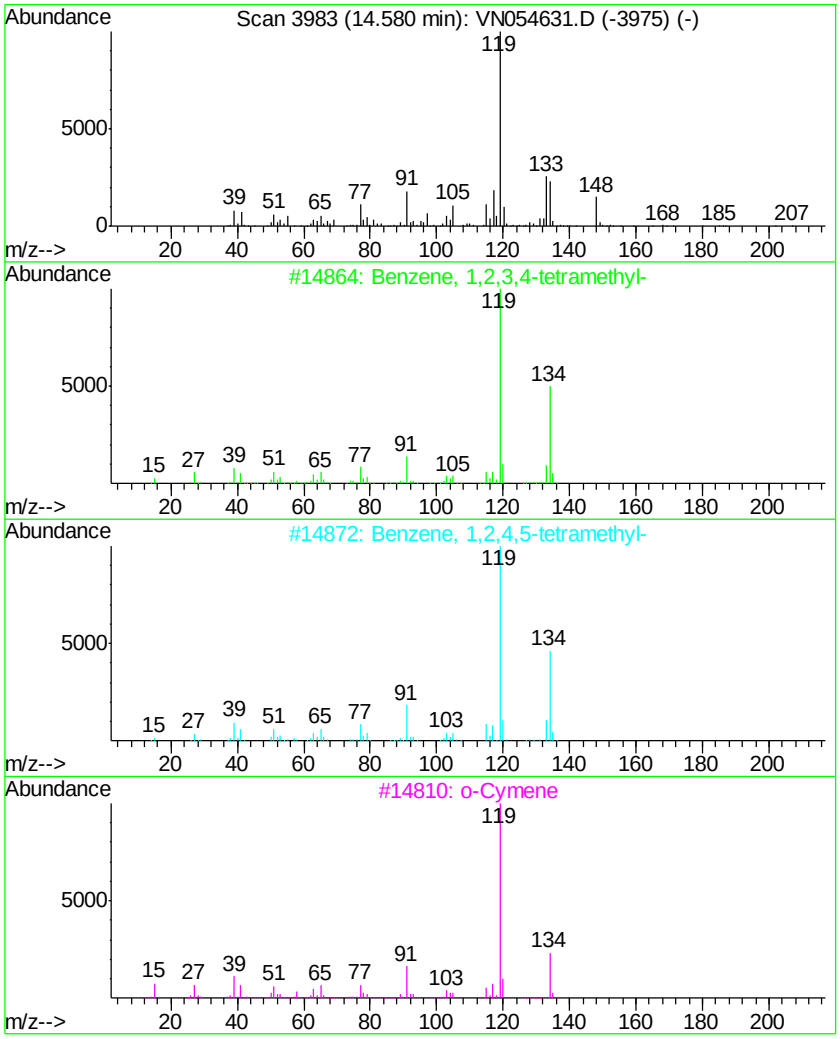
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

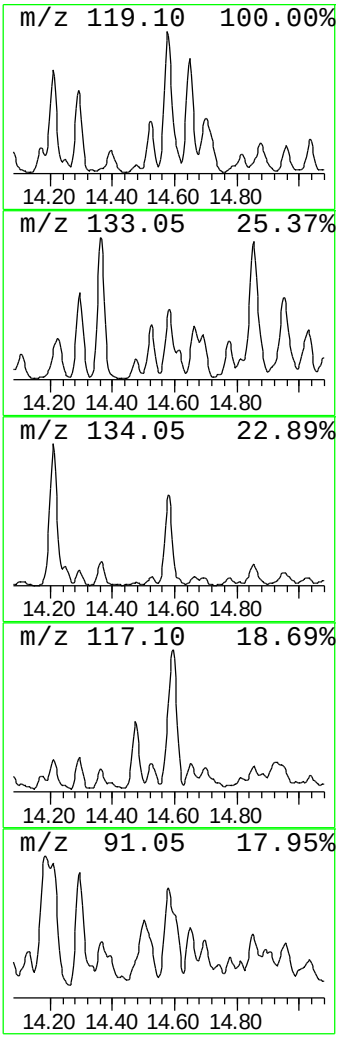
****

Peak Number 9 Benzene, 1,2,3,4-tetramethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.58	18.43 ug/l	998012	1,4-Dichlorobenzene-d4	13.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	64
2	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	64
3	o-Cymene	134	C10H14	000527-84-4	60
4	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	60
5	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	60





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN032319\
Data File : VN054631.D
Acq On : 24 Mar 2019 4:20
Operator : JC/SP
Sample : K2043-12
Misc : 6.52g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 39 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : WP022SB443-190319-(16-18)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N032019W.M
Quant Title : SW846 8260

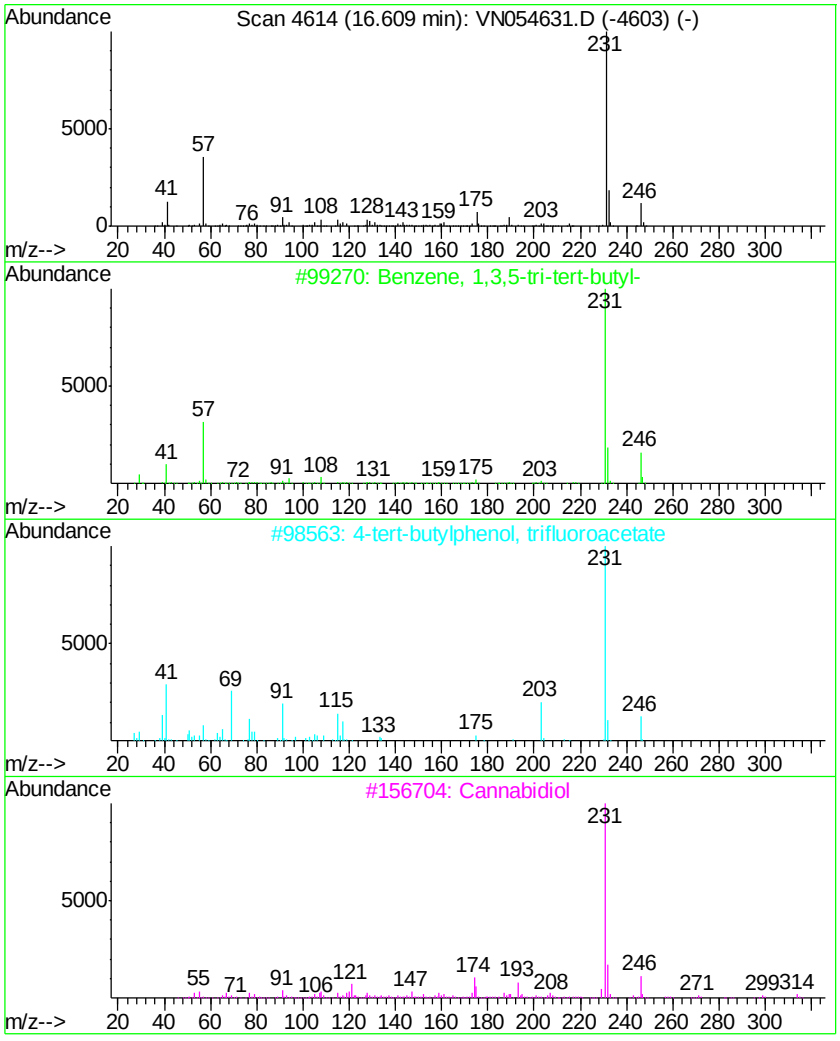
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

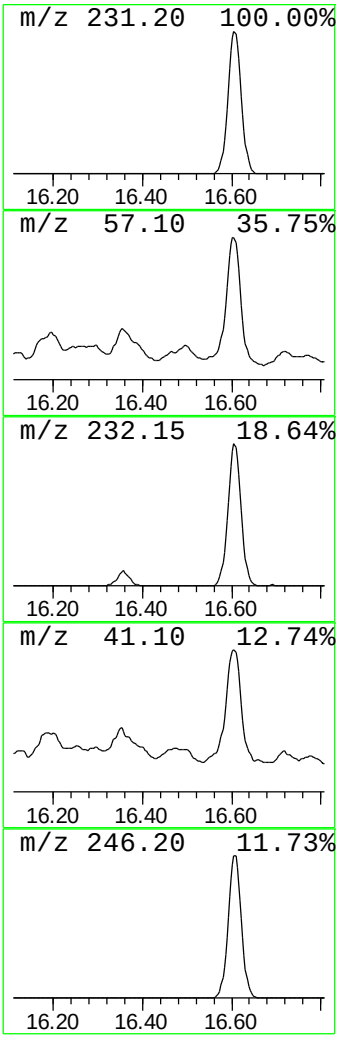
****

Peak Number 10 Benzene, 1,3,5-tri-tert-butyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.61	23.82 ug/l	1289330	1,4-Dichlorobenzene-d4	13.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,3,5-tri-tert-butyl-	246	C18H30	001460-02-2	87
2	4-tert-butylphenol, trifluoroace...	246	C12H13F3O2	1000376-51-5	72
3	Cannabidiol	314	C21H30O2	013956-29-1	56
4	2-Cyano-3-phenylquinoxaline	231	C15H9N3	059393-45-2	53
5	4-Methoxy-3-nitrophenyl methyl s...	231	C8H9NO5S	020945-69-1	53





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN032319\
Data File : VN054631.D
Acq On : 24 Mar 2019 4:20
Operator : JC/SP
Sample : K2043-12
Misc : 6.52g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 39 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : WP022SB443-190319-(16-18)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N032019W.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
unknown12.16	12.16	13.6	ug/l	1535410	3 11.41	5644480	50.0
1-Methyl-4-(1-met...	12.64	22.7	ug/l	1226610	4 13.34	2706910	50.0
Cyclohexane, 1,4-...	12.73	59.5	ug/l	3221710	4 13.34	2706910	50.0
Cyclohexane, 1-et...	12.78	18.0	ug/l	975838	4 13.34	2706910	50.0
Cyclohexane, butyl-	13.24	54.6	ug/l	2953600	4 13.34	2706910	50.0
Cyclohexane, pentyl-	14.18	69.3	ug/l	3751270	4 13.34	2706910	50.0
N-Methyl-o-toluamide	14.30	16.3	ug/l	880672	4 13.34	2706910	50.0
1-Methyldecahydro...	14.33	12.5	ug/l	677918	4 13.34	2706910	50.0
Benzene, 1,2,3,4-...	14.58	18.4	ug/l	998012	4 13.34	2706910	50.0
Benzene, 1,3,5-tr...	16.61	23.8	ug/l	1289330	4 13.34	2706910	50.0