LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN090718\
Data File : VN051053.D
Acq On : 7 Sep 2018 15:01
Operator : MD\SY
Sample : J4693-13
Misc : 5.92g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : EP1-MW-C(20-25)

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	1788	1809	1820	rBV	422687	1051092	34.06%	3.755%
2	7.664	1820	1832	1860	rVB	643032	1539418	49.88%	5.499%
3	8.027	1925	1945	1970	rBV	405152	955305	30.95%	3.413%
4	8.259	1991	2017	2022	rBV6	13809	47942	1.55%	0.171%
5	8.583	2102	2118	2140	rBV	909588	1894088	61.37%	6.766%
6	10.091	2570	2587	2620	rBV	1650789	3086190	100.00%	11.025%
7	10.432	2684	2693	2706	rVB4	19500	36171	1.17%	0.129%
8	10.718	2769	2782	2791	rBV3	26228	44611	1.45%	0.159%
9	10.818	2800	2813	2824	rBV4	14412	32428	1.05%	0.116%
10	11.005	2861	2871	2882	rVB2	75730	129541	4.20%	0.463%
11	11.124	2896	2908	2916	rBV3	42923	77506	2.51%	0.277%
12	11.210	2926	2935	2951	rVB2	72946	132932	4.31%	0.475%
13	11.406	2981	2996	3015	rBV	1249841	2224933	72.09%	7.948%
14	11.541	3030	3038	3046	rBV3	36719	53816	1.74%	0.192%
15	11.596	3046	3055	3063	rBV5	30365	57259	1.86%	0.205%
16	11.654	3063	3073	3081	rBV4	120474	230594	7.47%	0.824%
17	11.696	3082	3086	3097	rVB2	93084	140355	4.55%	0.501%
18	11.760	3097	3106	3110	rBV3	22888	37416	1.21%	0.134%
19	11.812	3112	3122	3127	rBV3	25632	49181	1.59%	0.176%
20	11.850	3127	3134	3142	rVB3	72072	112913	3.66%	0.403%
21	11.924	3142	3157	3169	rBV5	232262	571906	18.53%	2.043%
22	12.043	3186	3194	3203	rVB	381011	545665	17.68%	1.949%
23	12.120	3208	3218	3223	rBV4	238181	432886	14.03%	1.546%
24	12.294	3265	3272	3283	rVB5	183657	353366	11.45%	1.262%
25	12.403	3294	3306	3317	rBV	1190643	1973312	63.94%	7.049%
26	12.490	3317	3333	3339	rBV7	128158	342193	11.09%	1.222%
27	12.561	3349	3355	3371	rVB4	355611	696701	22.57%	2.489%
28	12.648	3371	3382	3392	rBV9	174650	403193	13.06%	1.440%
29	12.728	3393	3407	3416	rVV4	474003	1204265	39.02%	4.302%
30	12.779	3418	3423	3434	rVB4	267312	421965	13.67%	1.507%
31	12.873	3444	3452	3458	rBV5	210352	310519	10.06%	1.109%
32	12.927	3465	3469	3472	rBV2	99904	101932	3.30%	0.364%
33	12.963	3472	3480	3492	rVB	1219110	1986421	64.36%	7.096%
34	13.027	3494	3500	3511	rVB5	109814	182115	5.90%	0.651%

LSC Area Percent Report

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Sample : J4693-13
Misc : 5.92g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : EP1-MW-C(20-25)

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	13.088	3512	3519	3528	rBV2	183798	285702	9.26%	1.021%
36	13.146	3530	3537	3551	rVB7	218950	521673	16.90%	1.864%
37	13.217	3552	3559	3560	rBV3	143829	156758	5.08%	0.560%
38	13.239	3562	3566	3573	rVB3	219212	265496	8.60%	0.948%
39	13.342	3588	3598	3611	rVB	1108013	1849446	59.93%	6.607%
40	13.664	3688	3698	3707	rBV6	406035	778407	25.22%	2.781%
41	13.776	3726	3733	3743	rBV9	116858	262773	8.51%	0.939%
42	13.834	3745	3751	3760	rVV7	179384	376148	12.19%	1.344%
43	13.885	3762	3767	3776	rVV	277708	418945	13.57%	1.497%
44	13.934	3776	3782	3792	rVB2	173277	263511	8.54%	0.941%
45	13.992	3793	3800	3810	rVB5	151593	252068	8.17%	0.900%
46	14.175	3848	3857	3866	rBV5	162139	317744	10.30%	1.135%
47	14.332	3899	3906	3915	rBV4	116744	166959	5.41%	0.596%
48	14.586	3975	3985	3995	rBV2	167950	323333	10.48%	1.155%
49	14.641	3995	4002	4015	rVB3	145536	256003	8.30%	0.915%
50	15.117	4145	4150	4167	rVB4	17747	37471	1.21%	0.134%

Sum of corrected areas: 27992567

LSC Report - Integrated Chromatogram

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Data File : VN051053.D
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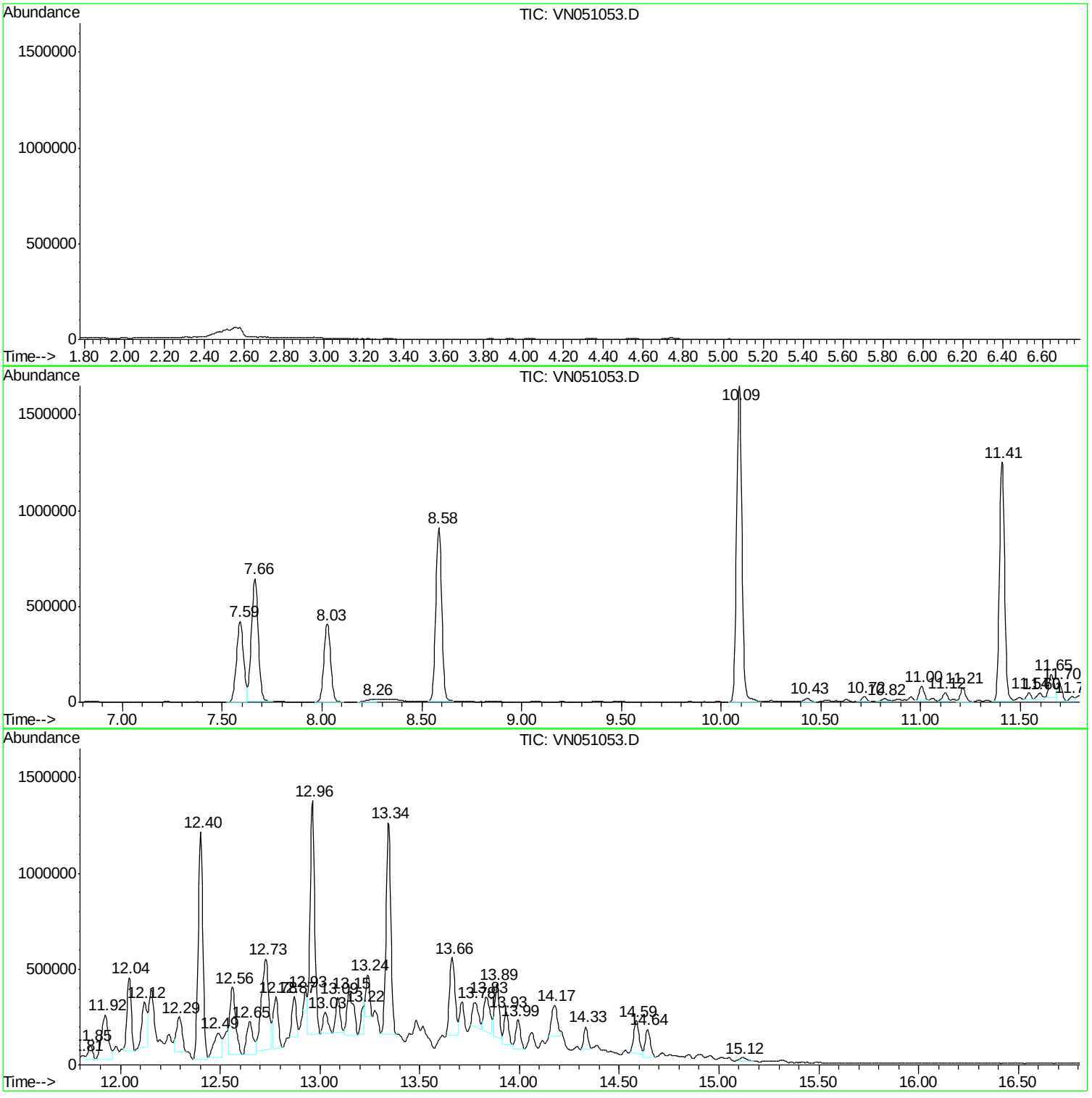
Operator : MD\SY
Sample : J4693-13
Misc : 5.92g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : EP1-MW-C(20-25)

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



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN090718\
Data File : VN051053.D
Acq On : 7 Sep 2018 15:01
Operator : MD\SY
Sample : J4693-13
Misc : 5.92g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : EP1-MW-C(20-25)

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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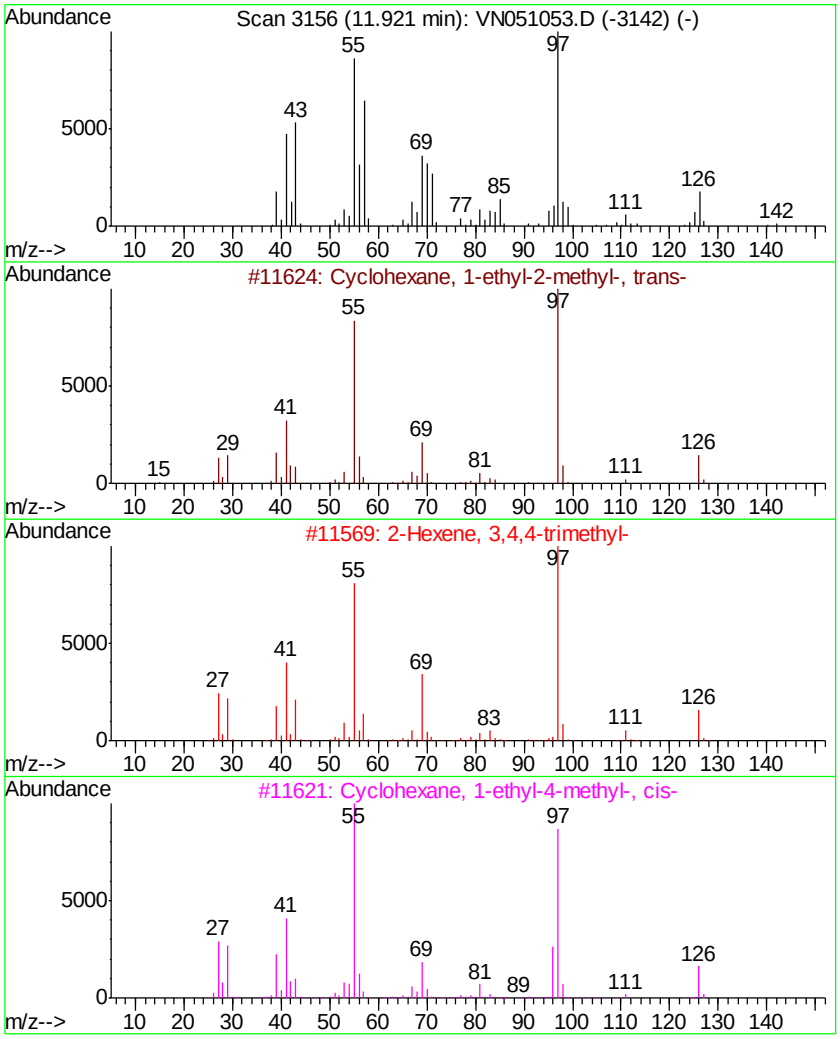
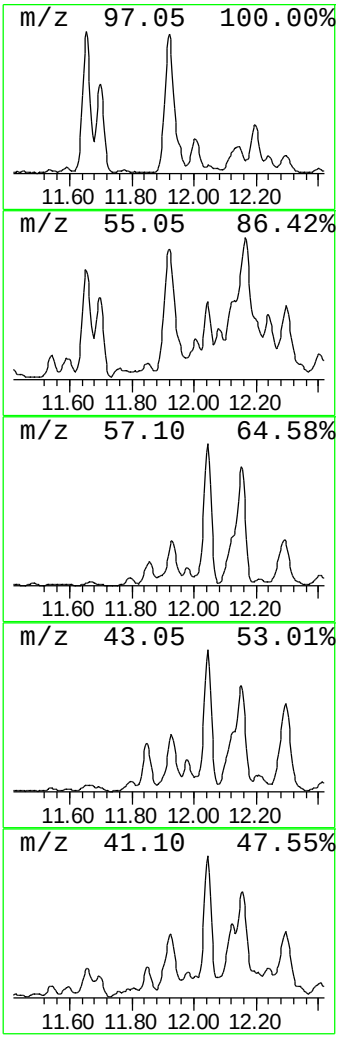
Peak Number 1 Cyclohexane, 1-ethyl-2-meth... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	12.85 ug/l	571906	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-78-8	45
2	2-Hexene, 3,4,4-trimethyl-	126	C9H18	053941-19-8	43
3	Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	004926-78-7	43
4	4-Octen-3-one	126	C8H14O	014129-48-7	38
5	3,5-Dimethyl-3-heptene	126	C9H18	059643-68-4	38





Library Search Compound Report

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Data File : VN051053.D
Acq On : 7 Sep 2018 15:01
Operator : MD\SY
Sample : J4693-13
Misc : 5.92g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : EP1-MW-C(20-25)

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

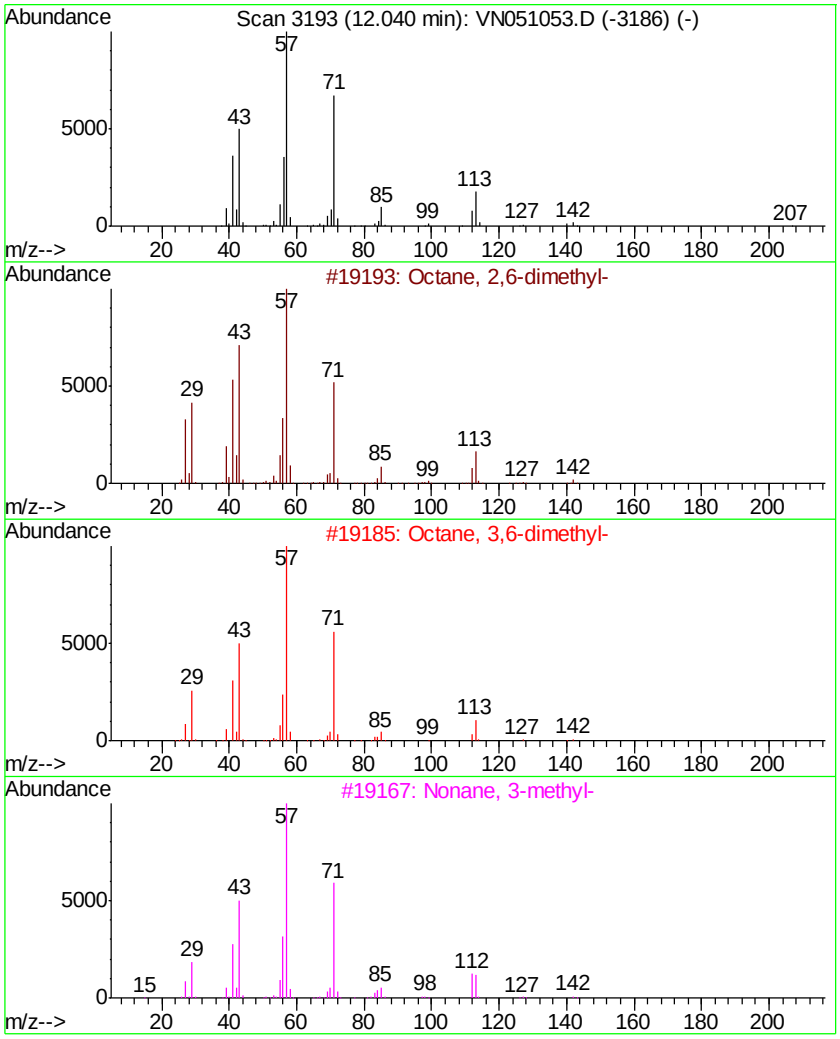
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

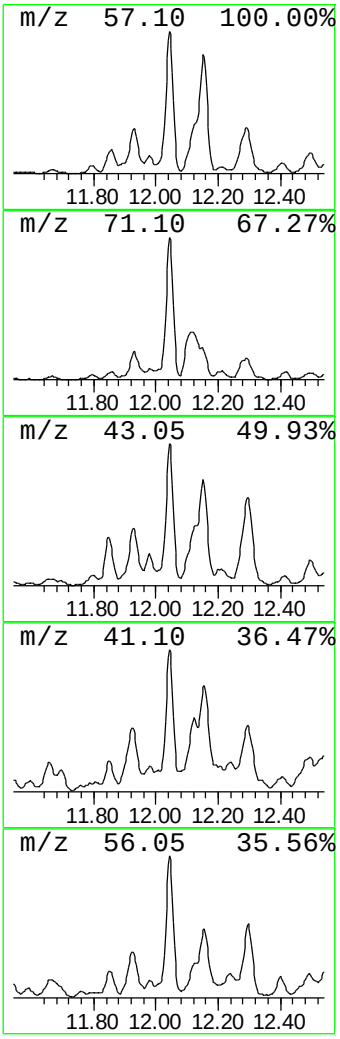
****

Peak Number 2 Octane, 2,6-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.04	12.26 ug/l	545665	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	Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	91
3	Nonane, 3-methyl-	142	C10H22	005911-04-6	87
4	Undecane, 6,6-dimethyl-	184	C13H28	017312-76-4	64
5	Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	53





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN090718\
Data File : VN051053.D
Acq On : 7 Sep 2018 15:01
Operator : MD\SY
Sample : J4693-13
Misc : 5.92g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : EP1-MW-C(20-25)

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

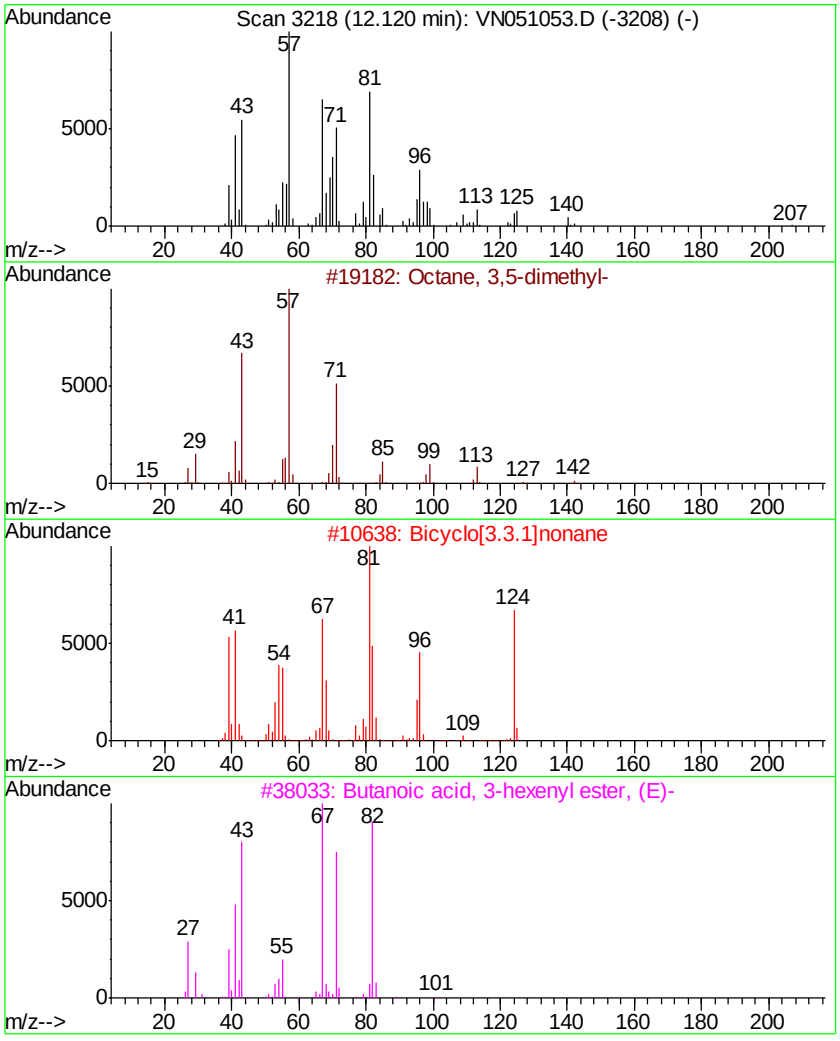
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

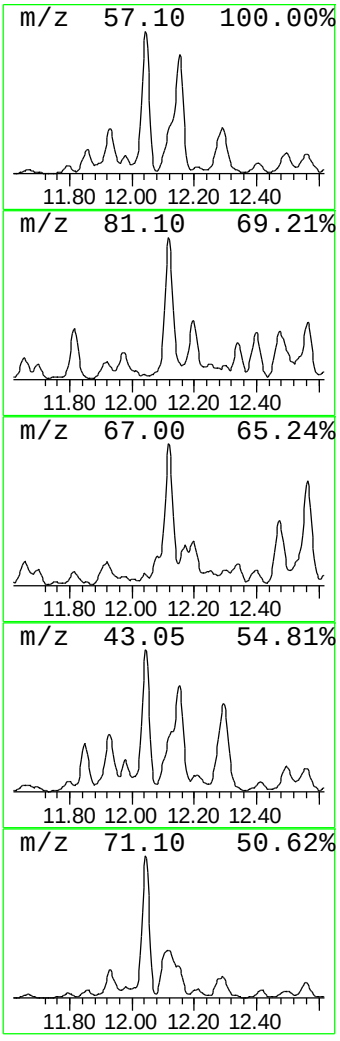
****

Peak Number 3 Octane, 3,5-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.12	9.73 ug/l	432886	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	42
2	Bicyclo[3.3.1]nonane	124	C9H16	000280-65-9	38
3	Butanoic acid, 3-hexenyl ester, ...	170	C10H18O2	053398-84-8	38
4	Cyclopropane, (2-methylenebutyl)-	110	C8H14	074685-56-6	38
5	1H-Indene, octahydro-, trans-	124	C9H16	003296-50-2	38





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN090718\
Data File : VN051053.D
Acq On : 7 Sep 2018 15:01
Operator : MD\SY
Sample : J4693-13
Misc : 5.92g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : EP1-MW-C(20-25)

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

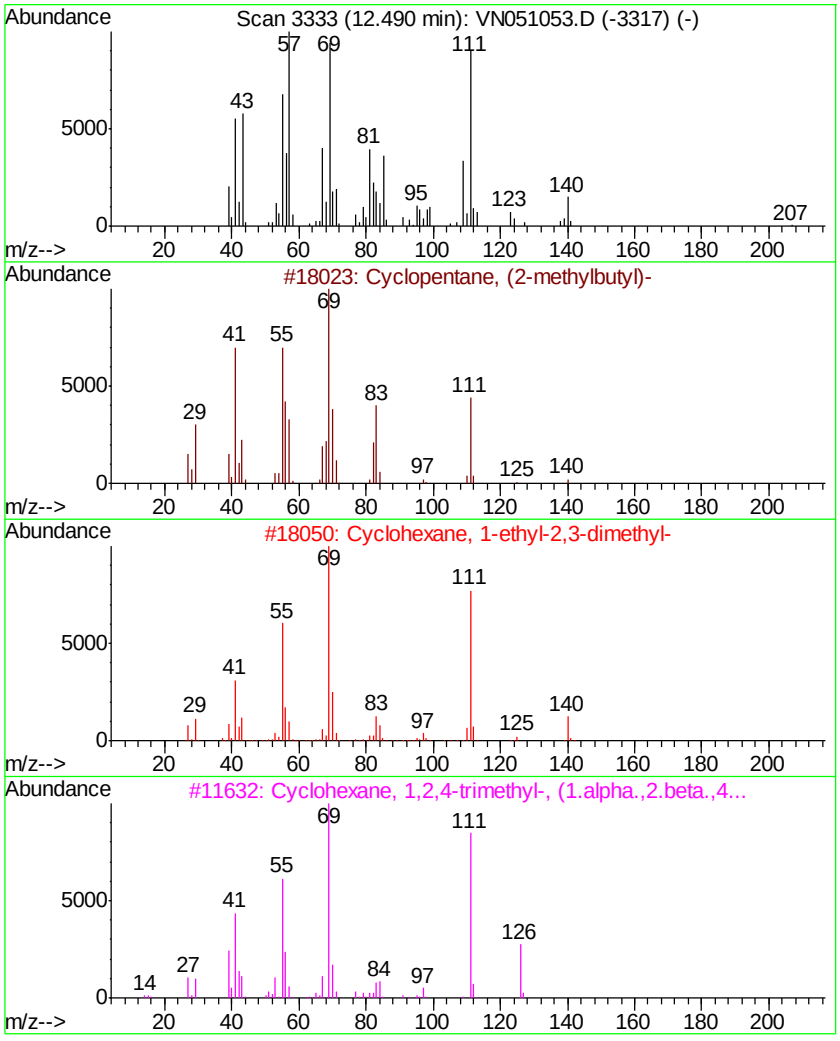
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

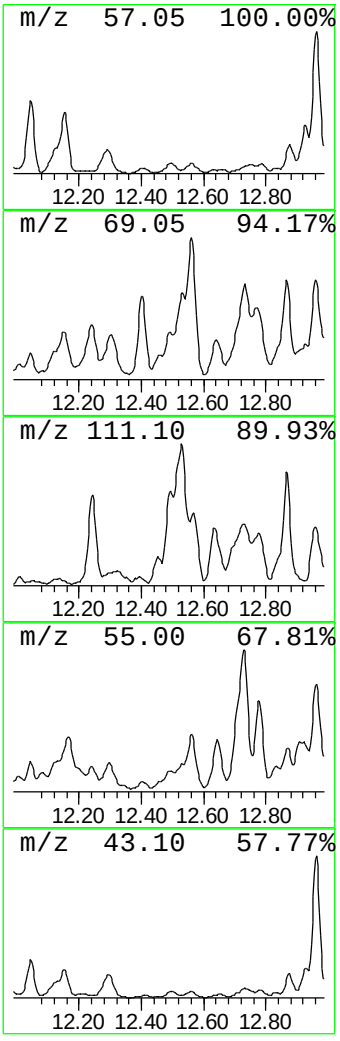
****

Peak Number 4 Cyclopentane, (2-methylbutyl)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.49	9.25 ug/l	342193	1,4-Dichlorobenzene-d4	13.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, (2-methylbutyl)-	140	C10H20	053366-38-4	58
2	Cyclohexane, 1-ethyl-2,3-dimethyl-	140	C10H20	007058-05-1	52
3	Cyclohexane, 1,2,4-trimethyl-, (...	126	C9H18	007667-60-9	47
4	2,4,6-Trimethyl-1,5-diazabicyclo...	126	C7H14N2	1000283-21-2	47
5	Cyclooctane, (1-methylpropyl)-	168	C12H24	016538-89-9	47





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ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : EP1-MW-C(20-25)

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

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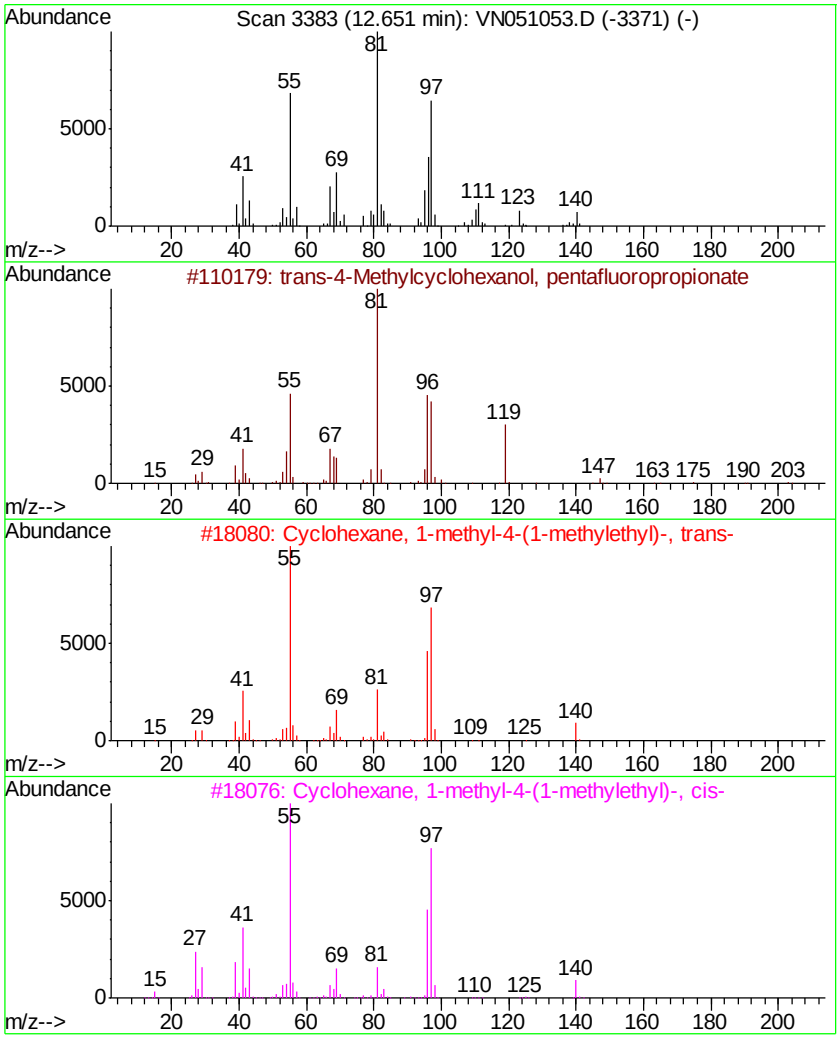
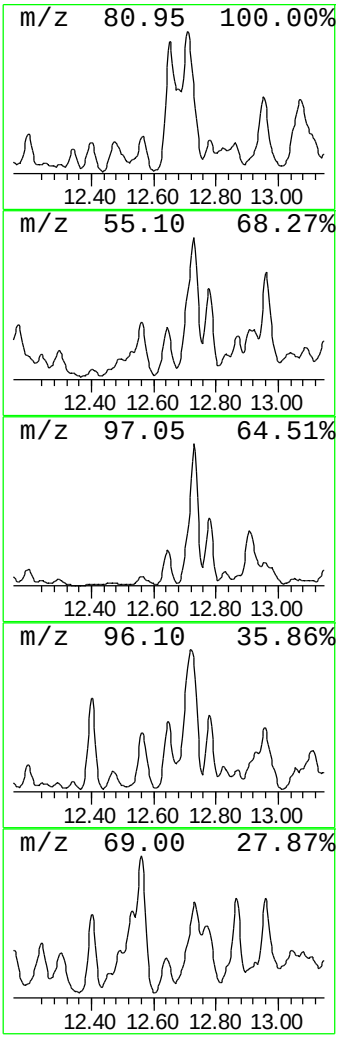
****

Peak Number 5 trans-4-Methylcyclohexanol,... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.65	10.90 ug/l	403193	1,4-Dichlorobenzene-d4	13.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-4-Methylcyclohexanol, pent...	260	C10H13F5O2	1000364-13-9	50
2	Cyclohexane, 1-methyl-4-(1-methy...	140	C10H20	001678-82-6	49
3	Cyclohexane, 1-methyl-4-(1-methy...	140	C10H20	006069-98-3	46
4	1-Methyl-4-(1-methylethyl)-cyclo...	140	C10H20	000099-82-1	46
5	Cyclohexene, 3-methyl-	96	C7H12	000591-48-0	43





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

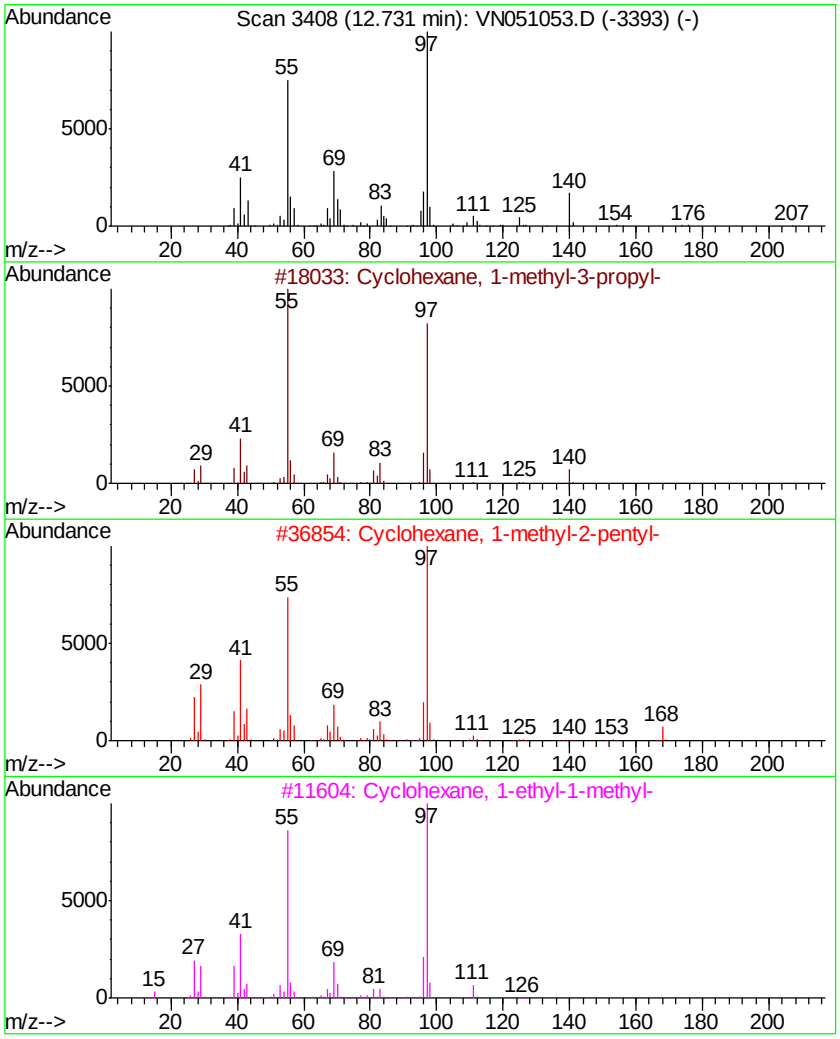
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

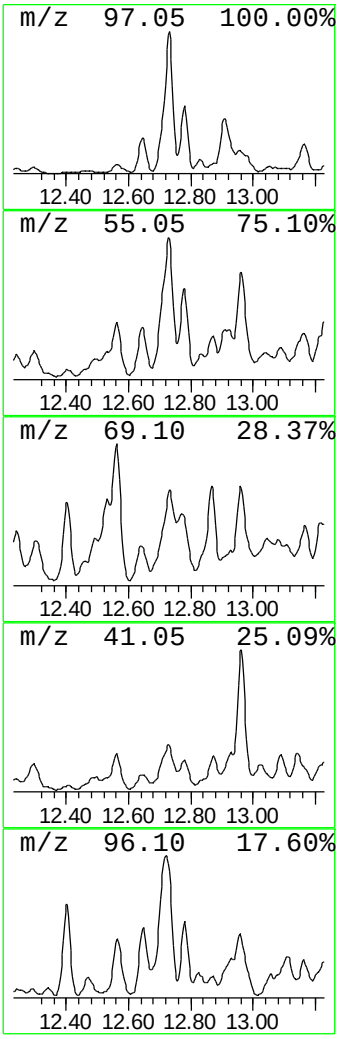
****

Peak Number 6 Cyclohexane, 1-methyl-3-pro... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.73	32.56 ug/l	1204270	1,4-Dichlorobenzene-d4	13.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1-methyl-3-propyl-	140	C10H20	004291-80-9	80
2	Cyclohexane, 1-methyl-2-pentyl-	168	C12H24	054411-01-7	72
3	Cyclohexane, 1-ethyl-1-methyl-	126	C9H18	004926-90-3	72
4	Cyclohexane, 1,1-dimethyl-	112	C8H16	000590-66-9	58
5	Cyclohexane, 1-methyl-4-(1-methy...	140	C10H20	001678-82-6	52





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Sample : J4693-13
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Instrument : MSVOA_N
ClientSampleId : EP1-MW-C(20-25)

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

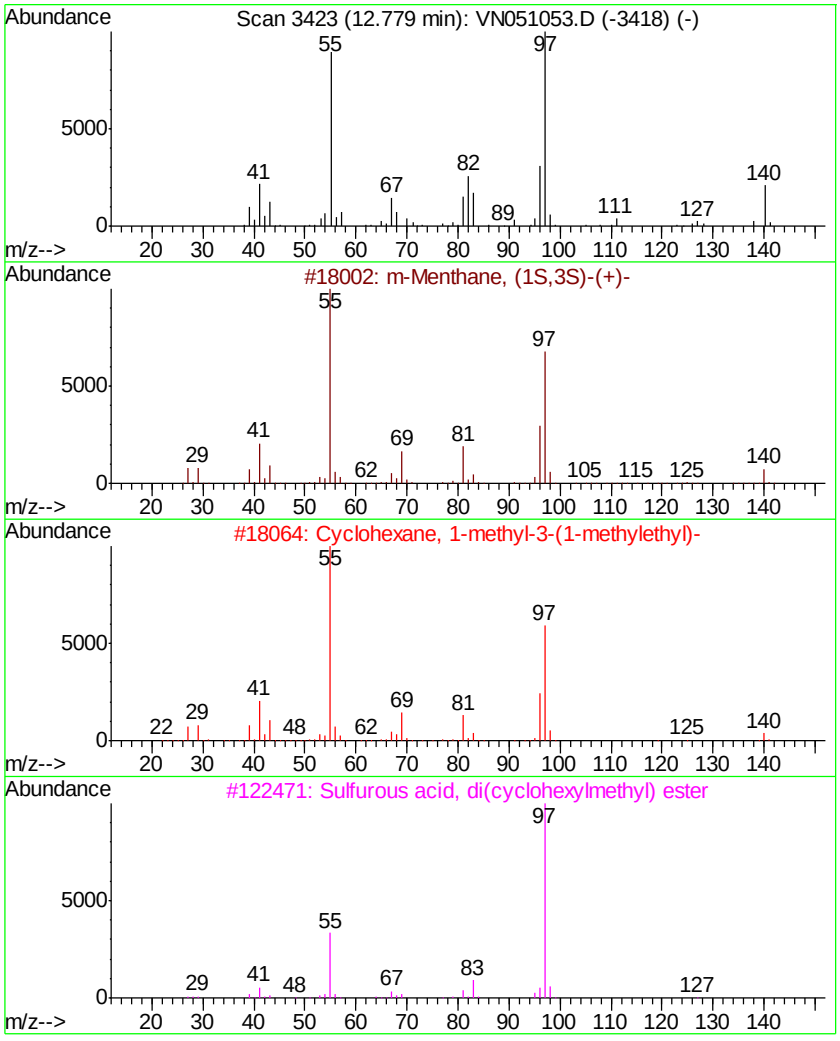
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

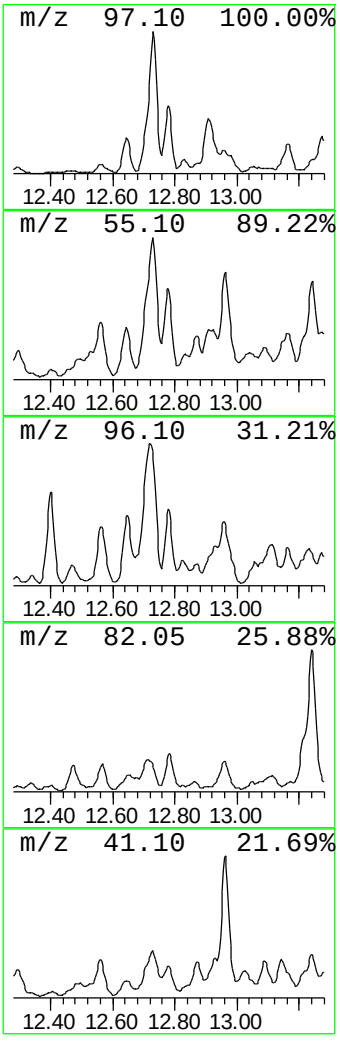
****

Peak Number 7 m-Menthane, (1S,3S)-(+)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.78	11.41 ug/l	421965	1,4-Dichlorobenzene-d4	13.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	m-Menthane, (1S,3S)-(+)-	140	C10H20	013837-67-7	72
2	Cyclohexane, 1-methyl-3-(1-methy...	140	C10H20	016580-24-8	59
3	Sulfurous acid, di(cyclohexylmet...	274	C14H26O3S	1000309-22-7	53
4	Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	006236-88-0	50
5	Sulfurous acid, cyclohexylmethyl...	332	C18H36O3S	1000309-21-9	50





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Data File : VN051053.D
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ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : EP1-MW-C(20-25)

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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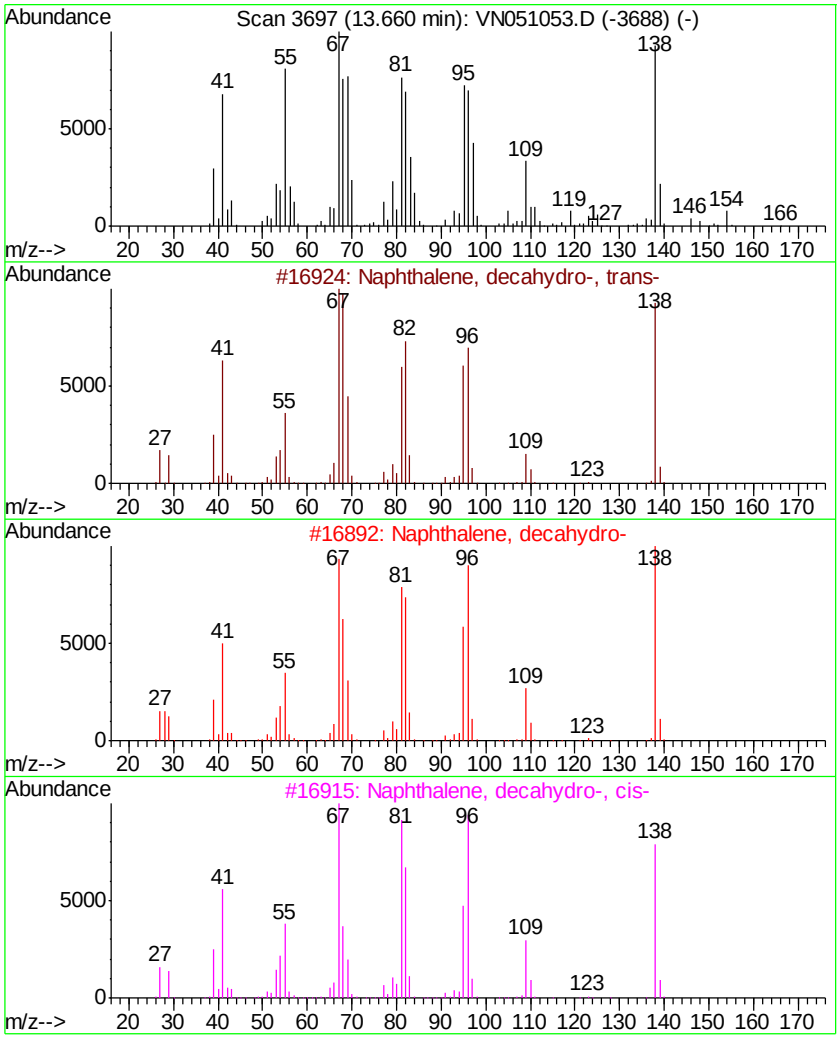
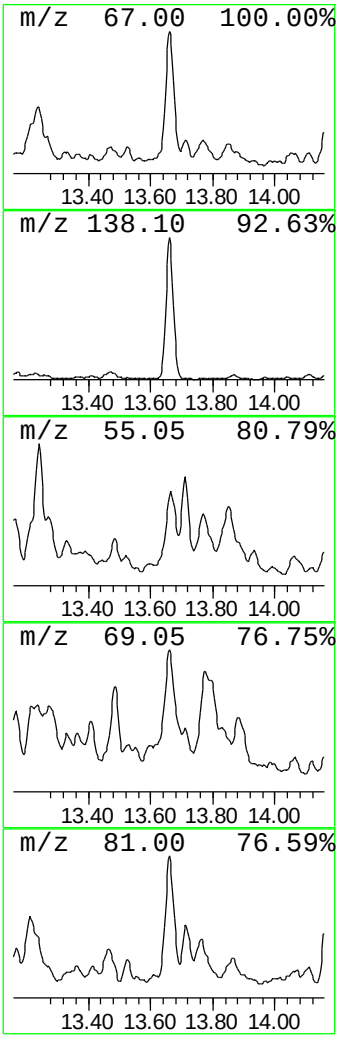
Peak Number 8 Naphthalene, decahydro-, tr... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.66	21.04 ug/l	778407	1,4-Dichlorobenzene-d4	13.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, decahydro-, trans-	138	C10H18	000493-02-7	93
2	Naphthalene, decahydro-	138	C10H18	000091-17-8	93
3	Naphthalene, decahydro-, cis-	138	C10H18	000493-01-6	90
4	Cyclohexane, 1-methyl-4-(1-methy...	138	C10H18	001124-25-0	64
5	Spiro[4.5]decane	138	C10H18	000176-63-6	58





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN090718\
Data File : VN051053.D
Acq On : 7 Sep 2018 15:01
Operator : MD\SY
Sample : J4693-13
Misc : 5.92g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : EP1-MW-C(20-25)

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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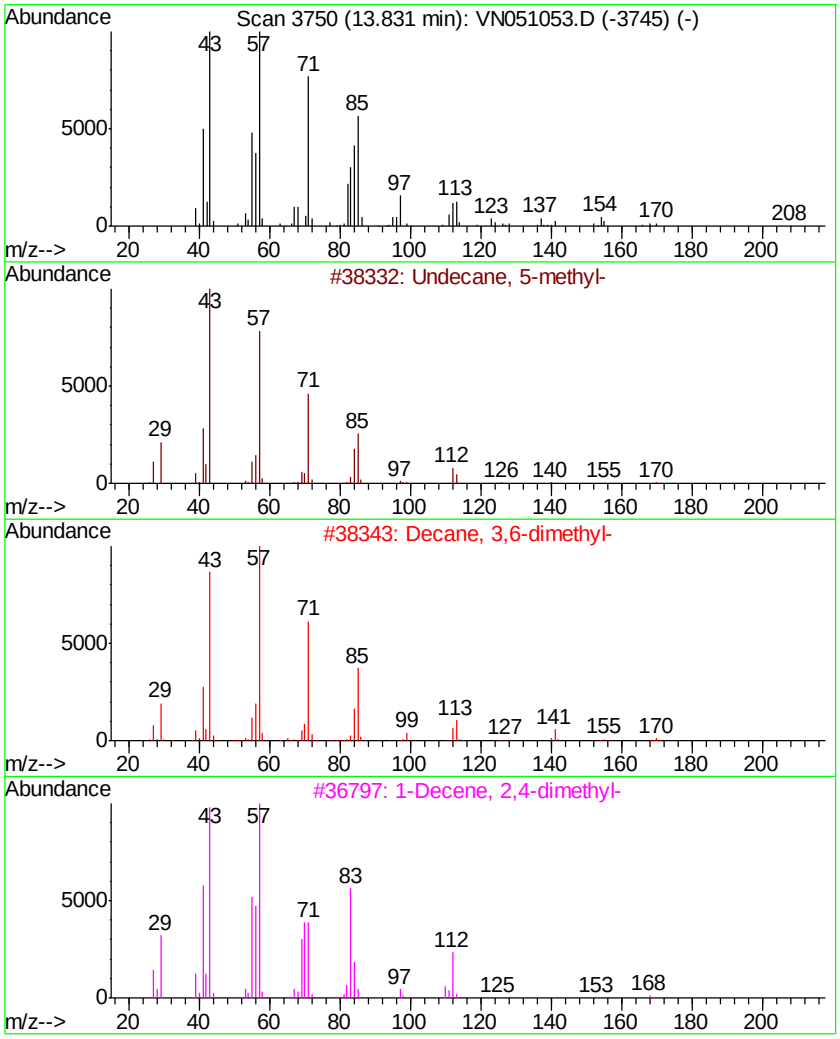
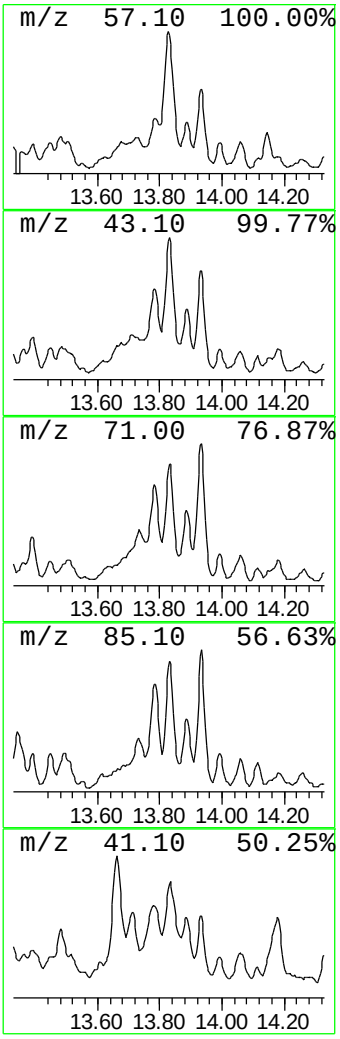
Peak Number 9 Undecane, 5-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	10.17 ug/l	376148	1,4-Dichlorobenzene-d4	13.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane, 5-methyl-	170	C12H26	001632-70-8	52
2	Decane, 3,6-dimethyl-	170	C12H26	017312-53-7	46
3	1-Decene, 2,4-dimethyl-	168	C12H24	055170-80-4	38
4	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	38
5	Heptane, 3-methyl-	114	C8H18	000589-81-1	35





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN090718\
Data File : VN051053.D
Acq On : 7 Sep 2018 15:01
Operator : MD\SY
Sample : J4693-13
Misc : 5.92g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : EP1-MW-C(20-25)

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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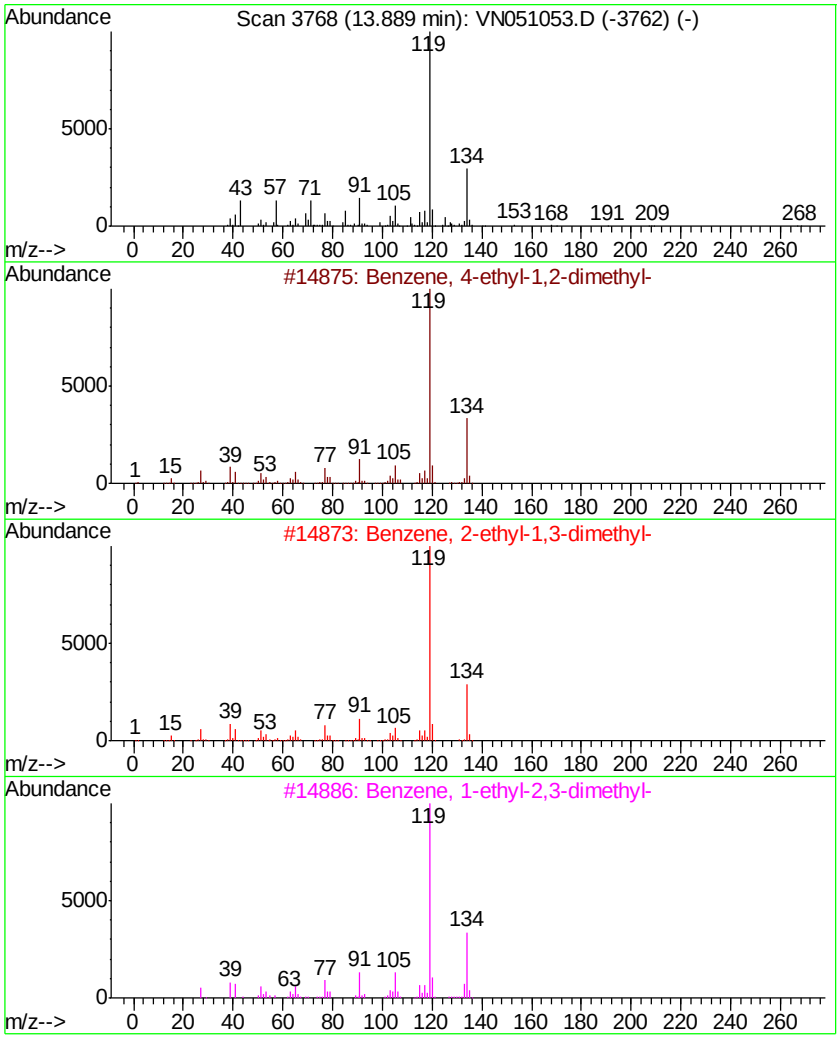
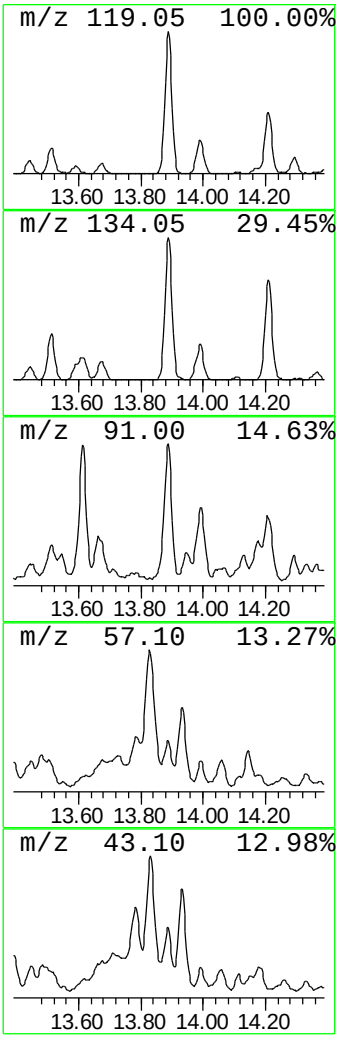
Peak Number 10 Benzene, 4-ethyl-1,2-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	11.33 ug/l	418945	1,4-Dichlorobenzene-d4	13.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	94
2	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	94
3	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	93
4	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	93
5	Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN090718\
Data File : VN051053.D
Acq On : 7 Sep 2018 15:01
Operator : MD\SY
Sample : J4693-13
Misc : 5.92g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : EP1-MW-C(20-25)

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-et...	11.92	12.9	ug/l	571906	3	11.41	2224930	50.0
Octane, 2,6-dimet...	12.04	12.3	ug/l	545665	3	11.41	2224930	50.0
Octane, 3,5-dimet...	12.12	9.7	ug/l	432886	3	11.41	2224930	50.0
Cyclopentane, (2-...	12.49	9.3	ug/l	342193	4	13.34	1849450	50.0
trans-4-Methylcyc...	12.65	10.9	ug/l	403193	4	13.34	1849450	50.0
Cyclohexane, 1-me...	12.73	32.6	ug/l	1204270	4	13.34	1849450	50.0
m-Menthane, (1S,3...	12.78	11.4	ug/l	421965	4	13.34	1849450	50.0
Naphthalene, deca...	13.66	21.0	ug/l	778407	4	13.34	1849450	50.0
Undecane, 5-methyl-	13.83	10.2	ug/l	376148	4	13.34	1849450	50.0
Benzene, 4-ethyl-...	13.89	11.3	ug/l	418945	4	13.34	1849450	50.0