LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN050219\
Data File : VN055353.D
Acq On : 2 May 2019 16:44
Operator : JC/SP
Sample : K2658-09 5X
Misc : 5.65g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : EP1-SB-E2-3(14-17)

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	8.587	2101	2119	2143	rBV	672965	1439322	1.37%	0.194%
2	10.088	2572	2586	2614	rBV2	1713541	3871377	3.69%	0.522%
3	10.432	2685	2693	2710	rVB	674800	1235353	1.18%	0.167%
4	10.718	2771	2782	2793	rVB	1419501	2401910	2.29%	0.324%
5	10.821	2793	2814	2826	rBV	832578	1915991	1.83%	0.258%
6	10.953	2845	2855	2862	rVV	2607136	4516641	4.30%	0.609%
7	11.005	2862	2871	2882	rVV2	3866855	6937160	6.61%	0.935%
8	11.124	2896	2908	2916	rBV5	1936447	3682591	3.51%	0.497%
9	11.204	2916	2933	2951	rVB7	5030152	12450183	11.86%	1.679%
10	11.300	2951	2963	2986	rBV	4732742	8730446	8.32%	1.177%
11	11.407	2986	2996	3004	rBV	931548	1707747	1.63%	0.230%
12	11.509	3015	3028	3034	rBV2	2536952	4849701	4.62%	0.654%
13	11.619	3045	3062	3069	rBV	7442623	18895280	18.00%	2.548%
14	11.696	3082	3086	3097	rVB3	4107775	6314335	6.02%	0.851%
15	11.757	3097	3105	3113	rBV2	750954	1397313	1.33%	0.188%
16	11.853	3129	3135	3142	rVB4	1027530	1489809	1.42%	0.201%
17	11.921	3142	3156	3170	rBV7	6497802	17306296	16.49%	2.334%
18	12.046	3187	3195	3201	rBV	5418405	7302481	6.96%	0.985%
19	12.120	3210	3218	3224	rBV2	5890636	9447715	9.00%	1.274%
20	12.165	3224	3232	3249	rVB5	11156201	22004479	20.97%	2.967%
21	12.249	3250	3258	3266	rBV	3799419	5745299	5.47%	0.775%
22	12.304	3267	3275	3280	rVV6	2454502	4594636	4.38%	0.620%
23	12.336	3281	3285	3300	rVB2	5408809	9526131	9.08%	1.284%
24	12.403	3301	3306	3313	rVB8	1283355	1762655	1.68%	0.238%
25	12.448	3313	3320	3327	rBV3	3274754	5539395	5.28%	0.747%
26	12.564	3348	3356	3360	rBV3	8258716	12868705	12.26%	1.735%
27	12.657	3373	3385	3391	rBV	29124730	49899738	47.54%	6.728%
28	12.734	3402	3409	3418	rVB2	29379445	48143759	45.87%	6.492%
29	12.783	3419	3424	3434	rVB2	5531700	8129044	7.75%	1.096%
30	12.892	3443	3458	3471	rBV3	10088383	22925495	21.84%	3.091%
31	12.963	3473	3480	3494	rVB4	7231952	12756712	12.15%	1.720%
32	13.043	3494	3505	3517	rBV2	62376292	104955601	100.00%	14.152%
33	13.169	3532	3544	3553	rBV2	6899239	14024041	13.36%	1.891%
34	13.236	3554	3565	3574	rVV3	16165474	29658511	28.26%	3.999%

LSC Area Percent Report

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Acq On : 2 May 2019 16:44
Operator : JC/SP
Sample : K2658-09 5X
Misc : 5.65g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : EP1-SB-E2-3(14-17)

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	13.287	3575	3581	3595	rVV2	7177905	11633118	11.08%	1.569%
36	13.378	3597	3609	3619	rVB2	28468161	46840249	44.63%	6.316%
37	13.541	3654	3660	3667	rVB	14273310	18396352	17.53%	2.481%
38	13.586	3667	3674	3690	rVB4	17118440	36281834	34.57%	4.892%
39	13.664	3690	3698	3709	rVB4	8128439	14345550	13.67%	1.934%
40	13.741	3714	3722	3732	rVB	6852675	9856467	9.39%	1.329%
41	13.802	3733	3741	3745	rBV	7657313	10780642	10.27%	1.454%
42	13.834	3746	3751	3759	rVB	8938441	12387582	11.80%	1.670%
43	13.889	3760	3768	3778	rVB	11728948	17867107	17.02%	2.409%
44	13.943	3778	3785	3791	rBV	1554757	2341311	2.23%	0.316%
45	13.995	3791	3801	3810	rVB3	11774602	19684055	18.75%	2.654%
46	14.050	3811	3818	3820	rBV2	1602466	2085300	1.99%	0.281%
47	14.127	3833	3842	3850	rBV2	4197254	6544727	6.24%	0.882%
48	14.178	3850	3858	3862	rVV3	2456425	4343806	4.14%	0.586%
49	14.207	3863	3867	3873	rVV	4173886	6049276	5.76%	0.816%
50	14.249	3874	3880	3887	rVB	6760618	9318098	8.88%	1.256%
51	14.294	3887	3894	3900	rBV2	2730278	3512998	3.35%	0.474%
52	14.332	3900	3906	3913	rVB2	2178880	2546893	2.43%	0.343%
53	14.432	3931	3937	3944	rVB2	2268402	3322666	3.17%	0.448%
54	14.477	3944	3951	3959	rVV4	1351612	2847988	2.71%	0.384%
55	14.522	3961	3965	3973	rVB2	2080735	2803425	2.67%	0.378%
56	14.580	3973	3983	3998	rBV3	7433940	15463619	14.73%	2.085%
57	14.648	3999	4004	4014	rVB2	936100	1400087	1.33%	0.189%
58	14.741	4024	4033	4043	rVB	3988160	6018850	5.73%	0.812%
59	14.850	4060	4067	4072	rBV5	757025	1082422	1.03%	0.146%
60	14.956	4091	4100	4117	rVB3	947500	2130292	2.03%	0.287%
61	15.130	4145	4154	4166	rVB	1905096	3319238	3.16%	0.448%

Sum of corrected areas: 741629804

LSC Report - Integrated Chromatogram

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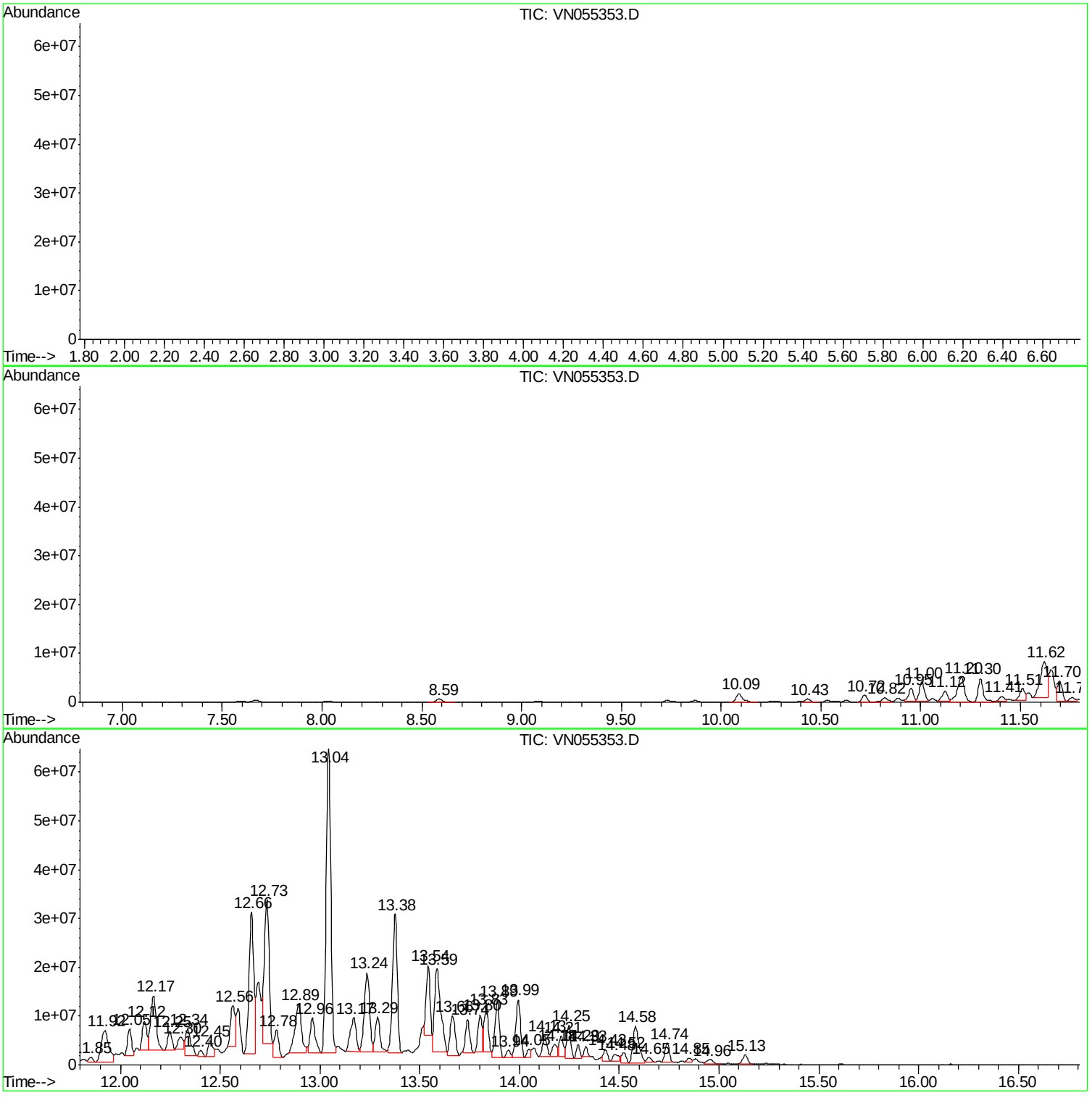
ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : EP1-SB-E2-3(14-17)

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



Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN050219\
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Acq On : 2 May 2019 16:44
Operator : JC/SP
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Instrument : MSVOA_N
ClientSampleId : EP1-SB-E2-3(14-17)

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

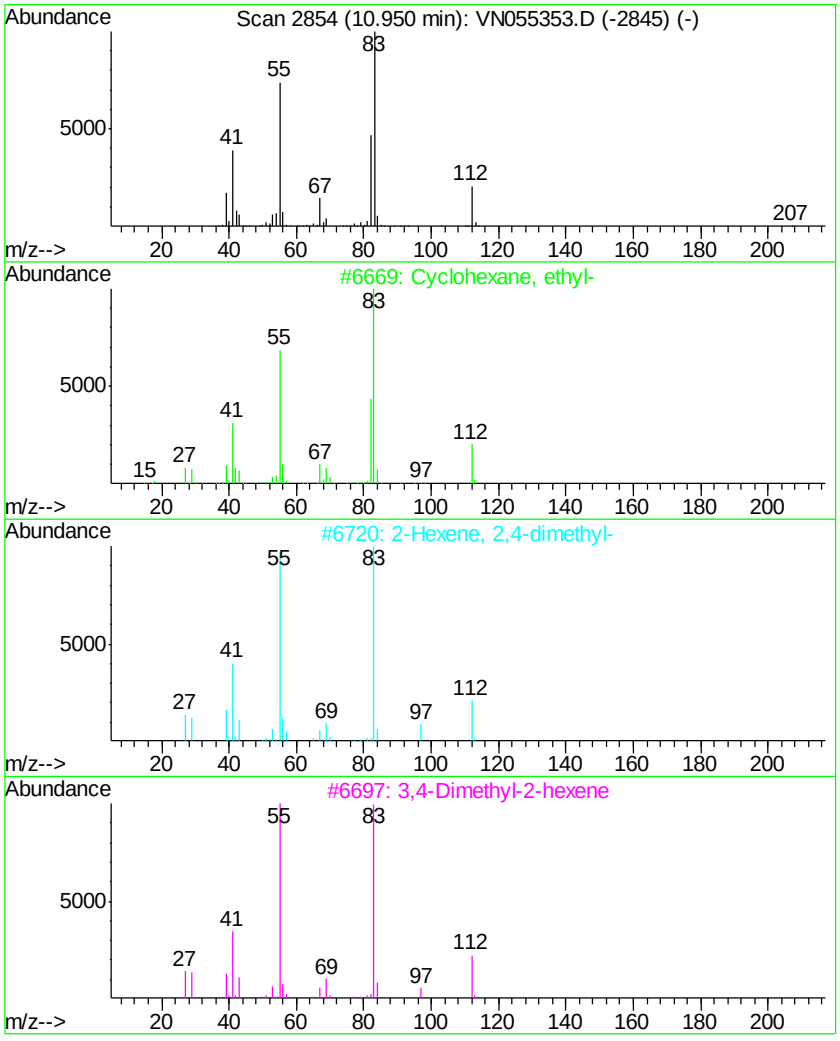
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

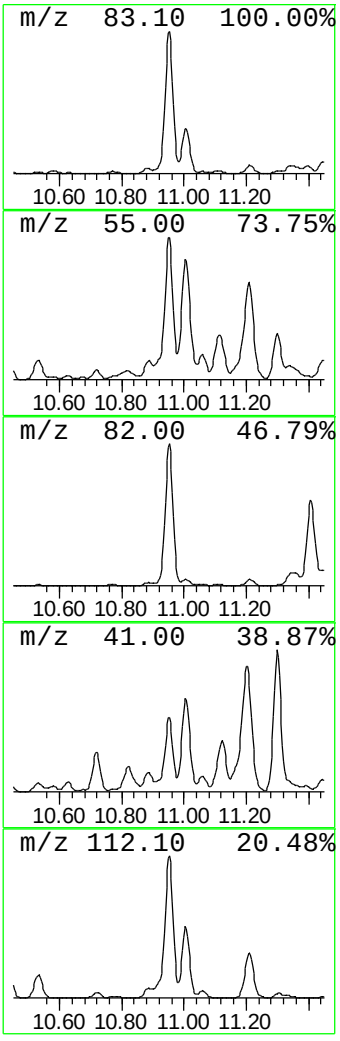
****

Peak Number 1 Cyclohexane, ethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.95	132.24 ug/l	4516640	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, ethyl-	112	C8H16	001678-91-7	87
2	2-Hexene, 2,4-dimethyl-	112	C8H16	014255-23-3	58
3	3,4-Dimethyl-2-hexene	112	C8H16	002213-37-8	58
4	trans-4,4-Dimethyl-2-hexene	112	C8H16	019550-83-5	53
5	4-Hexen-3-one, 5-methyl-	112	C7H12O	013905-10-7	53





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN050219\
Data File : VN055353.D
Acq On : 2 May 2019 16:44
Operator : JC/SP
Sample : K2658-09 5X
Misc : 5.65g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : EP1-SB-E2-3(14-17)

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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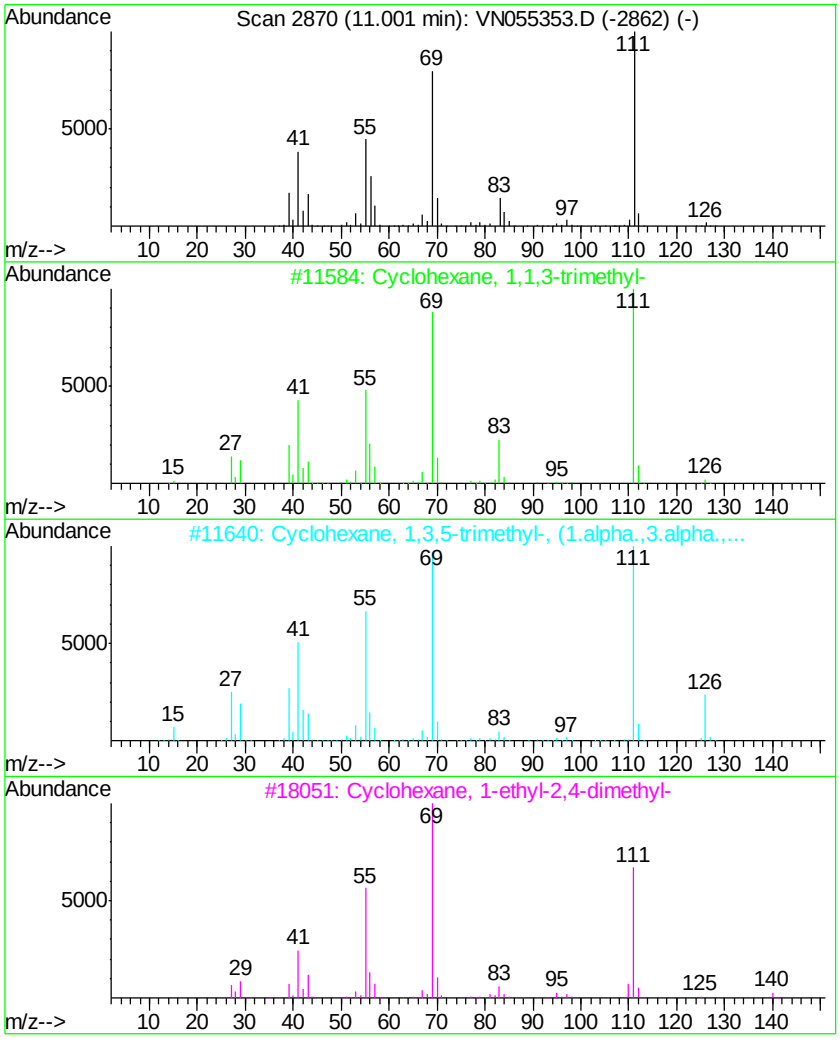
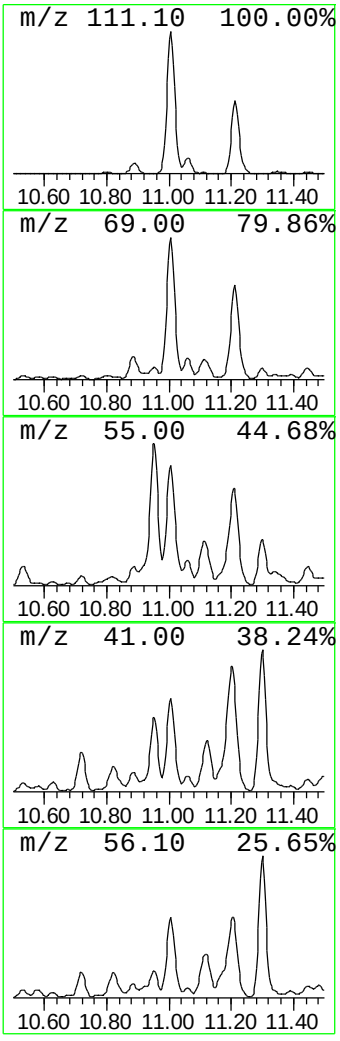
Peak Number 2 Cyclohexane, 1,1,3-trimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.00	203.11 ug/l	6937160	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,1,3-trimethyl-	126	C9H18	003073-66-3	90
2	Cyclohexane, 1,3,5-trimethyl-, (...	126	C9H18	001795-27-3	72
3	Cyclohexane, 1-ethyl-2,4-dimethyl-	140	C10H20	061142-69-6	72
4	Cyclohexane, 1,3,5-trimethyl-	126	C9H18	001839-63-0	72
5	Cyclohexane, 1,3,5-trimethyl-, (...	126	C9H18	001795-26-2	53





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN050219\
Data File : VN055353.D
Acq On : 2 May 2019 16:44
Operator : JC/SP
Sample : K2658-09 5X
Misc : 5.65g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
EP1-SB-E2-3(14-17)

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

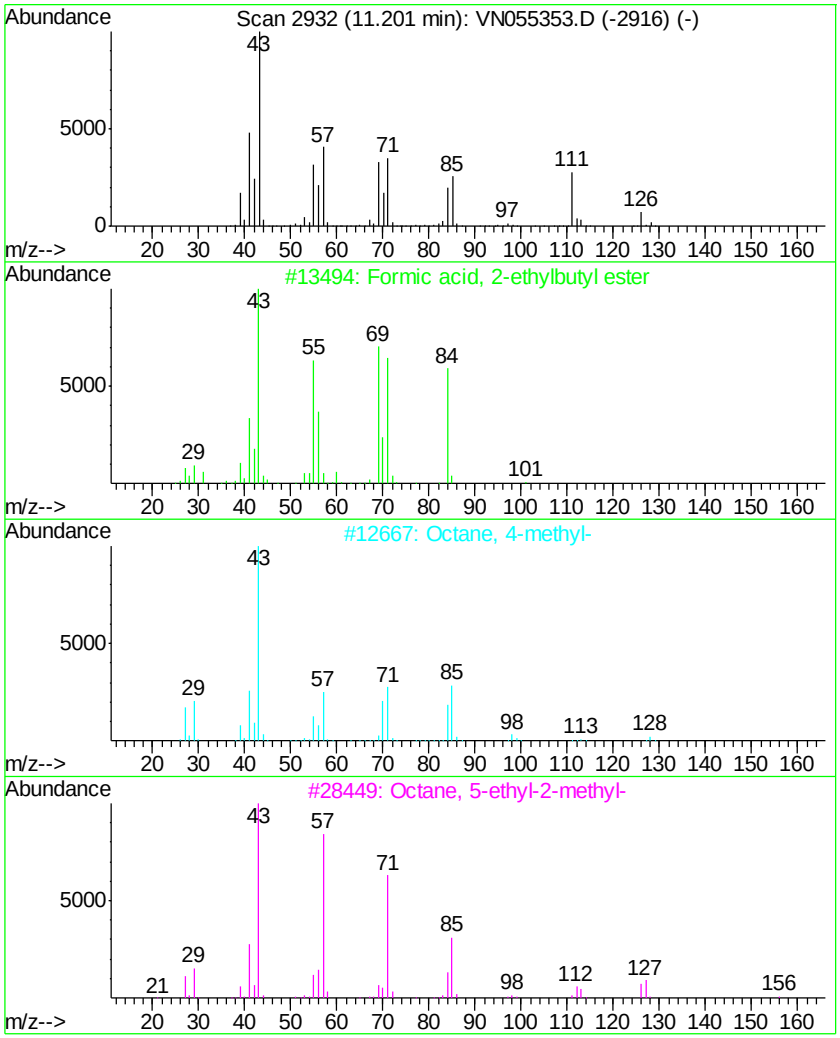
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

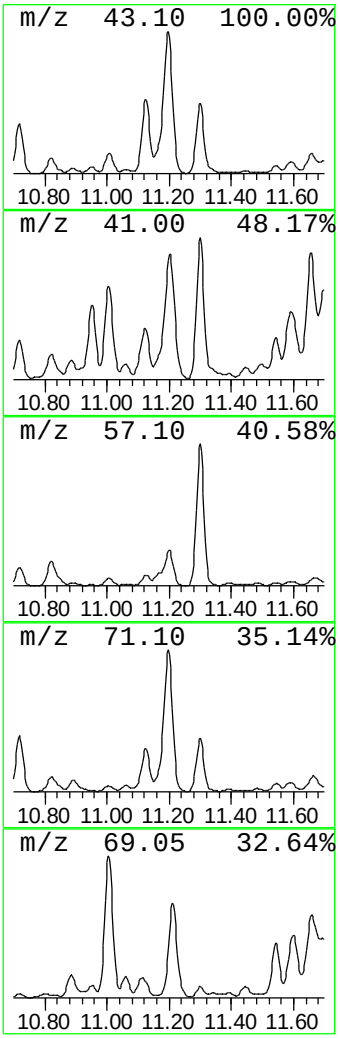
****

Peak Number 3 unknown11.20 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.20	364.52 ug/l	12450200	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Formic acid, 2-ethylbutyl ester	130	C7H14O2	1000367-92-2	35
2	Octane, 4-methyl-	128	C9H20	002216-34-4	35
3	Octane, 5-ethyl-2-methyl-	156	C11H24	062016-18-6	35
4	Silane, trichlorodocosyl-	442	C22H45Cl3Si	007325-84-0	35
5	Heptane, 3,4,5-trimethyl-	142	C10H22	020278-89-1	27





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN050219\
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Misc : 5.65g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : EP1-SB-E2-3(14-17)

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

TIC Library : C:\DATABASE\NIST11.L
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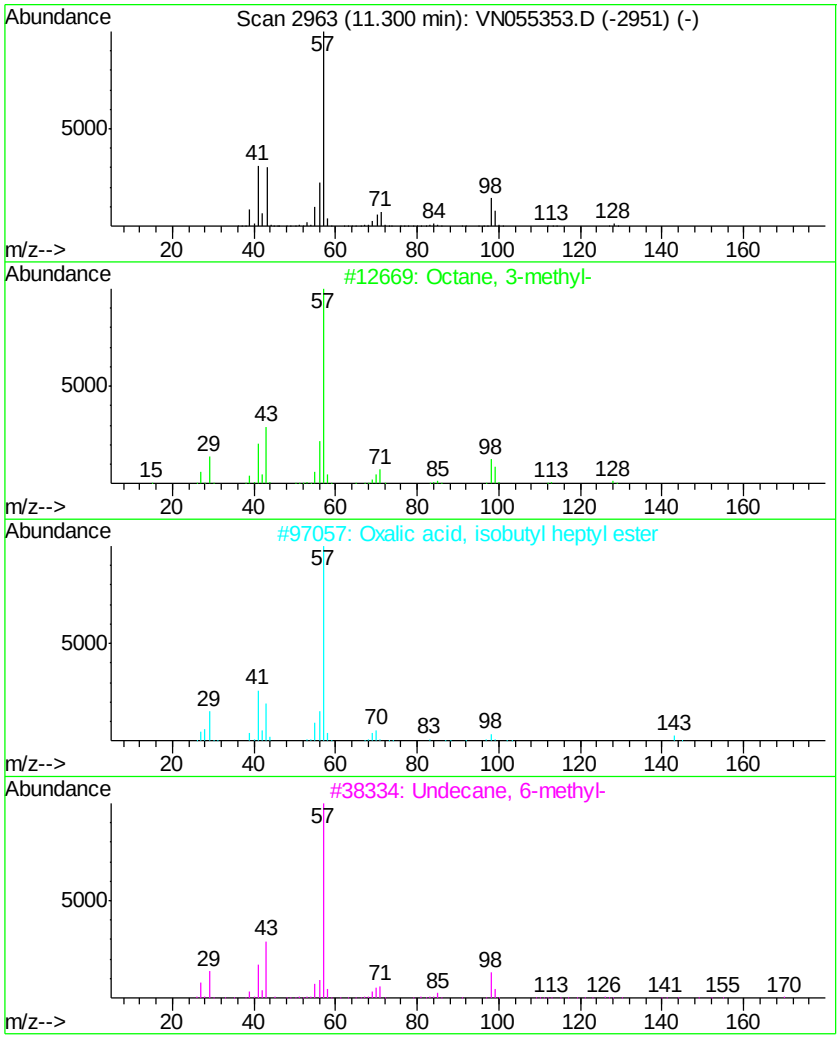
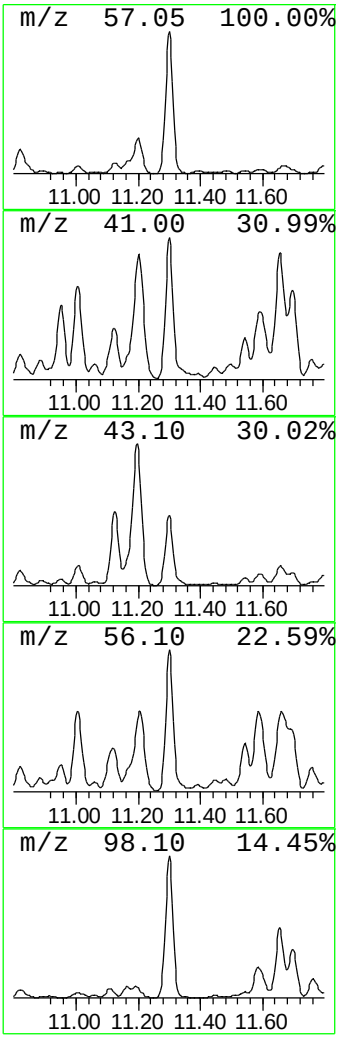
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.30	255.61 ug/l	8730450	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 3-methyl-	128	C9H20	002216-33-3	91
2	Oxalic acid, isobutyl heptyl ester	244	C13H24O4	1000309-37-2	64
3	Undecane, 6-methyl-	170	C12H26	017302-33-9	59
4	Heptane, 2,5-dimethyl-	128	C9H20	002216-30-0	59
5	Heptane, 4-(1-methylethyl)-	142	C10H22	052896-87-4	59





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Operator : JC/SP
Sample : K2658-09 5X
Misc : 5.65g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : EP1-SB-E2-3(14-17)

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

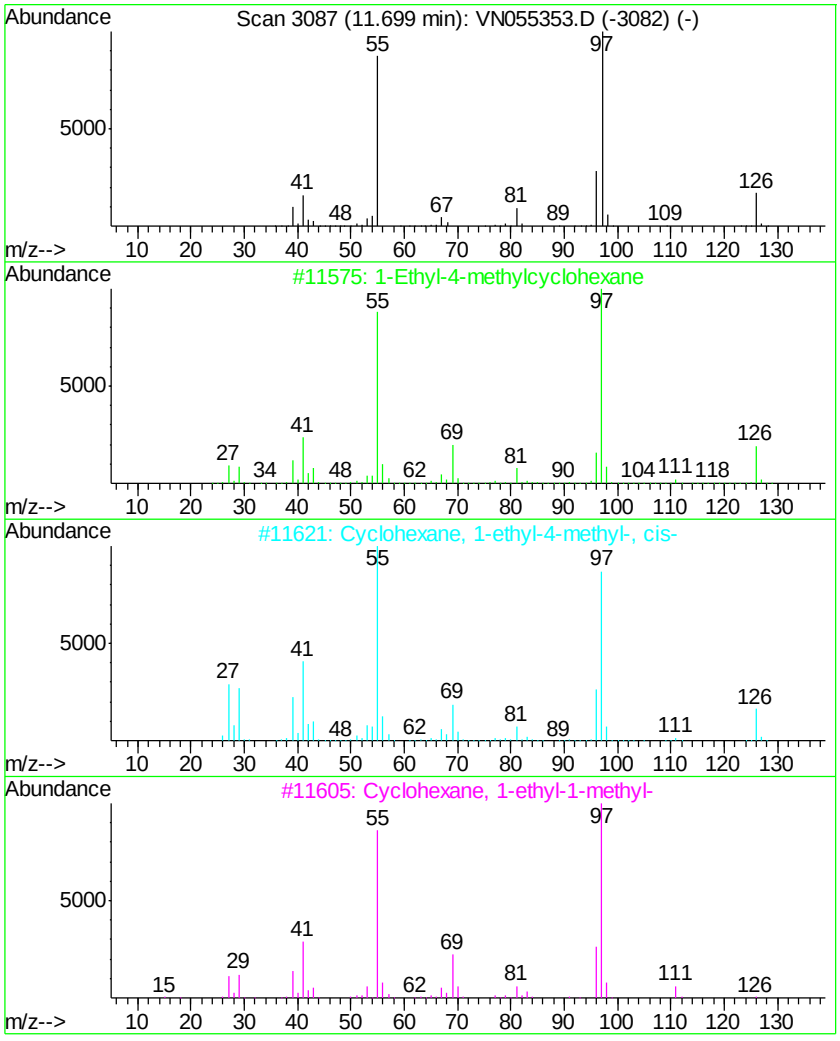
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

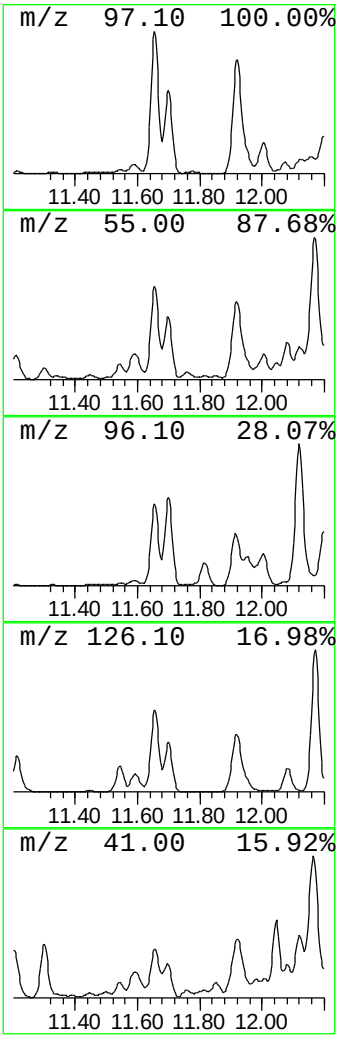
****

Peak Number 5 1-Ethyl-4-methylcyclohexane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.70	184.87 ug/l	6314340	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	86
3	Cyclohexane, 1-ethyl-1-methyl-	126	C9H18	004926-90-3	72
4	Cyclopentane, 1-hydroxymethyl-1,...	128	C8H16O	1000156-73-8	64
5	Cyclohexane, 1-bromo-4-methyl-	176	C7H13Br	006294-40-2	64





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Misc : 5.65g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : EP1-SB-E2-3(14-17)

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

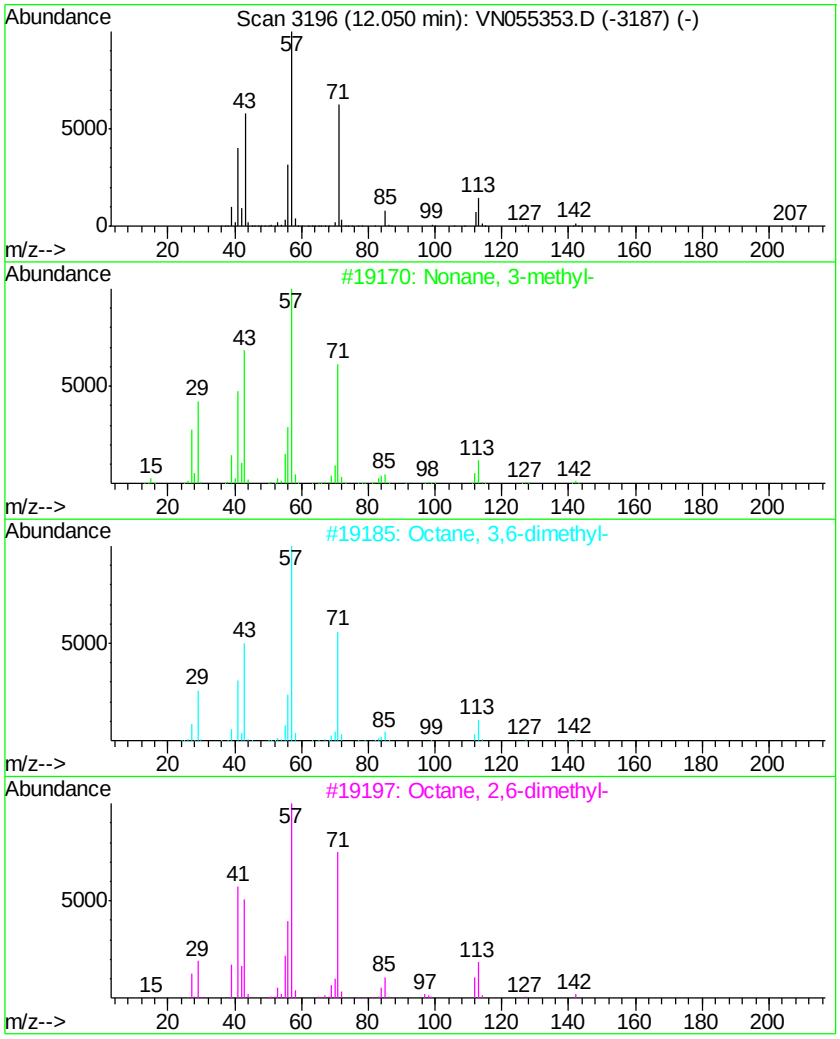
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

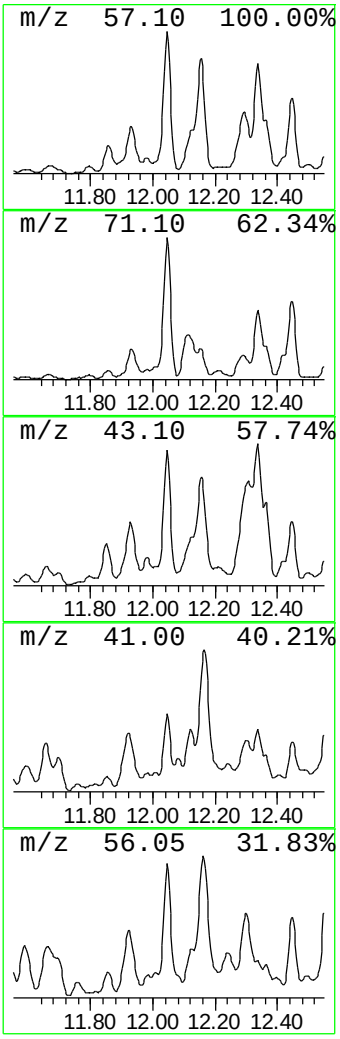
****

Peak Number 6 Nonane, 3-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.05	213.81 ug/l	7302480	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, 3,6-dimethyl-	142	C10H22	015869-94-0	91
3	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	90
4	Decane, 2,6,7-trimethyl-	184	C13H28	062108-25-2	64
5	Oxalic acid, isobutyl pentyl ester	216	C11H20O4	1000309-37-0	59





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN050219\
Data File : VN055353.D
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Operator : JC/SP
Sample : K2658-09 5X
Misc : 5.65g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : EP1-SB-E2-3(14-17)

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

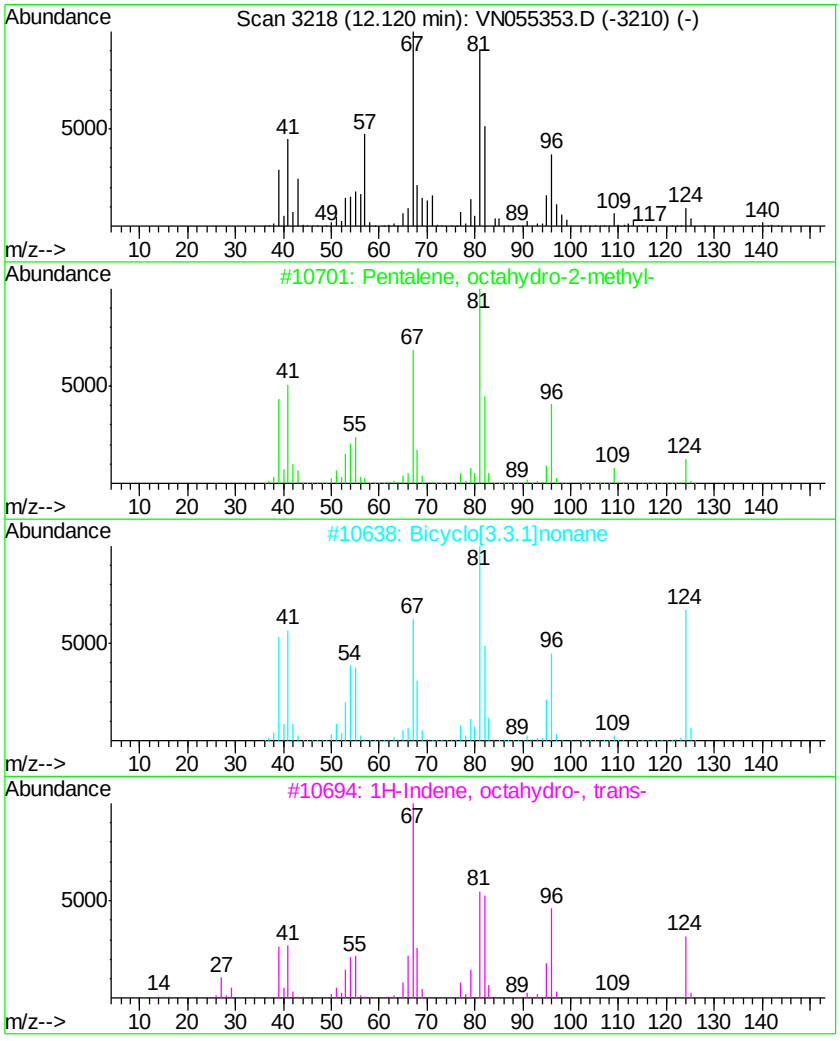
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

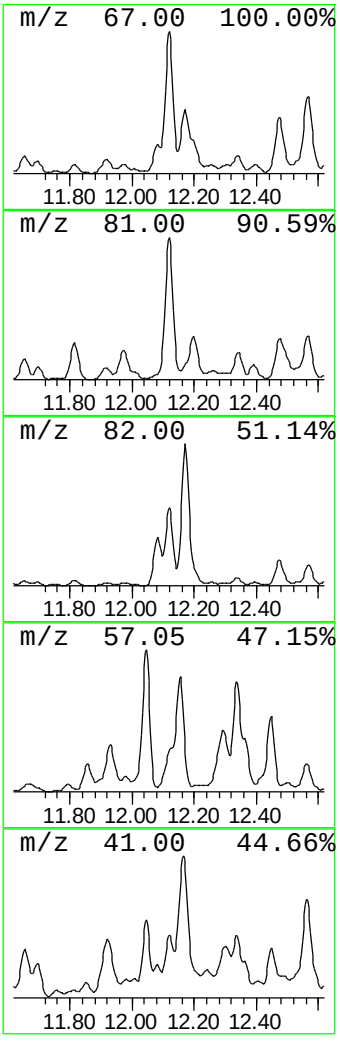
****

Peak Number 7 Pentalene, octahydro-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.12	276.61 ug/l	9447720	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	Bicyclo[3.3.1]nonane	124	C9H16	000280-65-9	58
3	1H-Indene, octahydro-, trans-	124	C9H16	003296-50-2	58
4	Cyclohexene,3-propyl-	124	C9H16	003983-06-0	46
5	Cyclohexene, 4-methyl-	96	C7H12	000591-47-9	46





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN050219\
Data File : VN055353.D
Acq On : 2 May 2019 16:44
Operator : JC/SP
Sample : K2658-09 5X
Misc : 5.65g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : EP1-SB-E2-3(14-17)

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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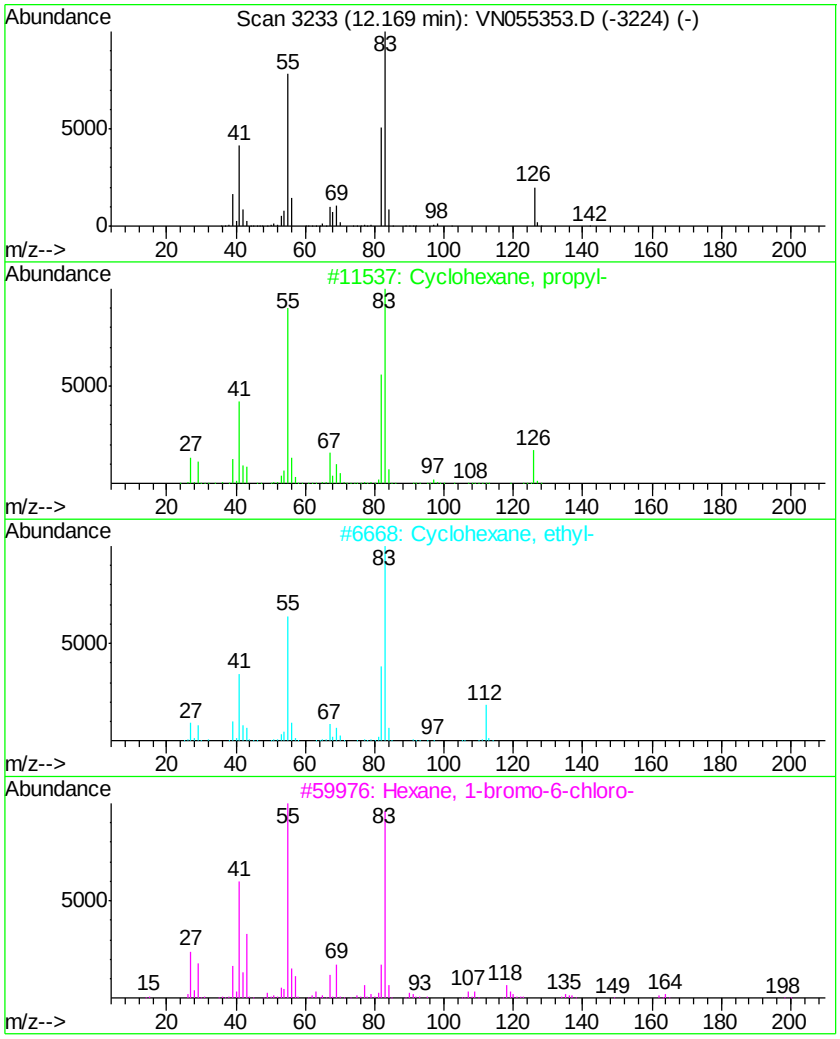
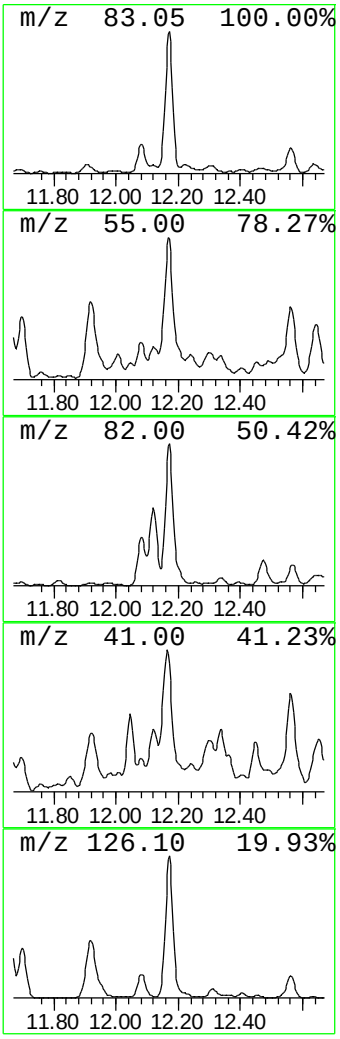
Peak Number 8 Cyclohexane, propyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.17	644.26 ug/l	22004500	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	Hexane, 1-bromo-6-chloro-	198	C6H12BrCl	006294-17-3	53
4	Cyclopentane, 1-ethyl-1-methyl-	112	C8H16	016747-50-5	53
5	Ethanone, 1-(1-methylcyclopentyl)-	126	C8H14O	013388-93-7	53





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN050219\
Data File : VN055353.D
Acq On : 2 May 2019 16:44
Operator : JC/SP
Sample : K2658-09 5X
Misc : 5.65g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : EP1-SB-E2-3(14-17)

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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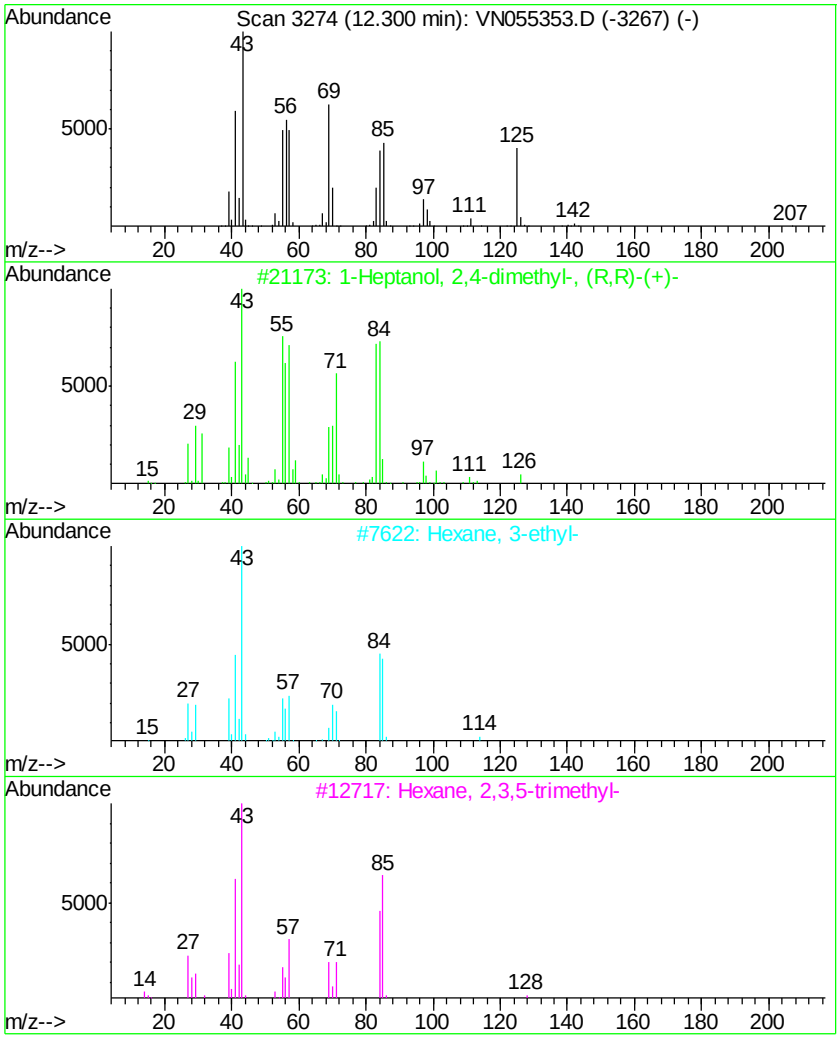
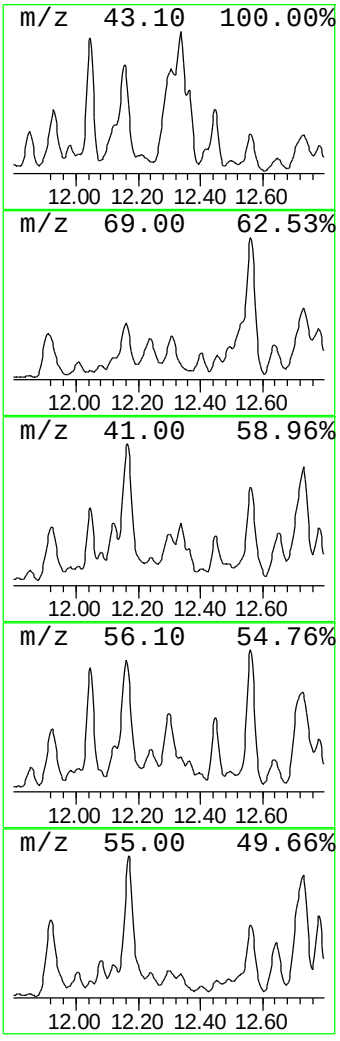
Peak Number 9 unknown12.30 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.30	134.52 ug/l	4594640	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptanol, 2,4-dimethyl-, (R,R)...	144	C9H20O	018450-73-2	38
2	Hexane, 3-ethyl-	114	C8H18	000619-99-8	35
3	Hexane, 2,3,5-trimethyl-	128	C9H20	001069-53-0	35
4	3-Ethyl-3-methyl-2-pentanol	130	C8H18O	066576-22-5	35
5	2(1H)-Pyridinone, 4-hydroxy-6-me...	125	C6H7NO2	003749-51-7	35





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN050219\
Data File : VN055353.D
Acq On : 2 May 2019 16:44
Operator : JC/SP
Sample : K2658-09 5X
Misc : 5.65g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : EP1-SB-E2-3(14-17)

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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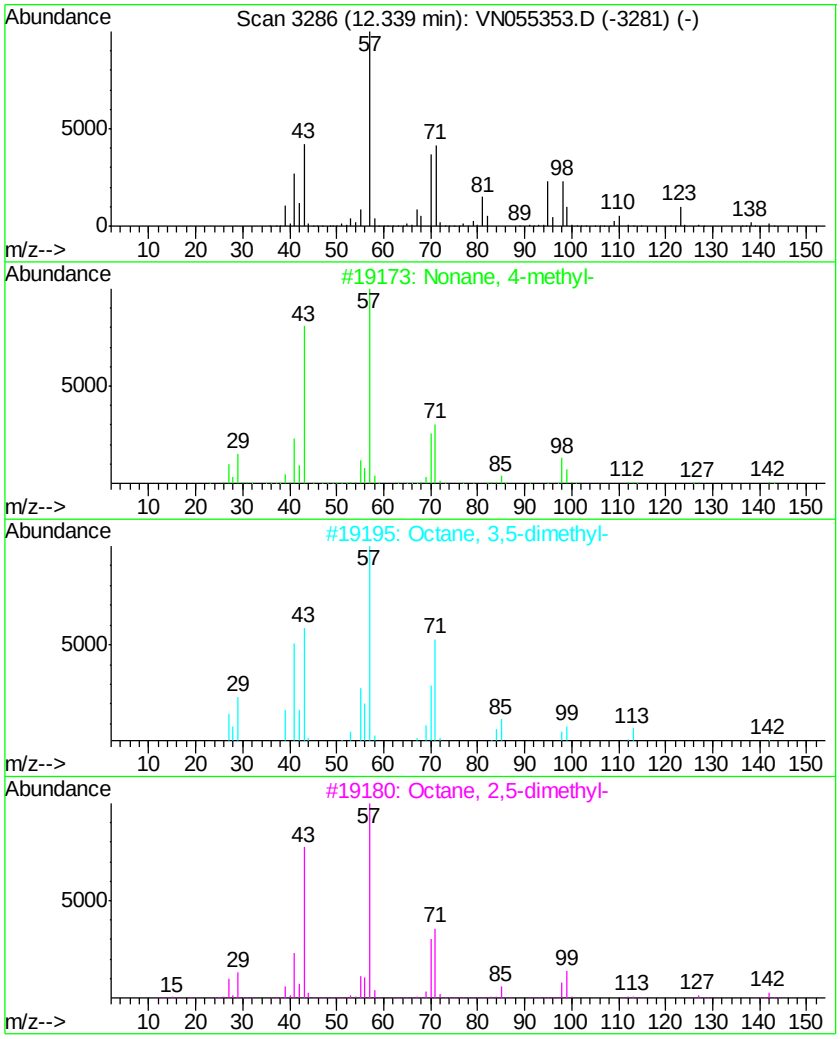
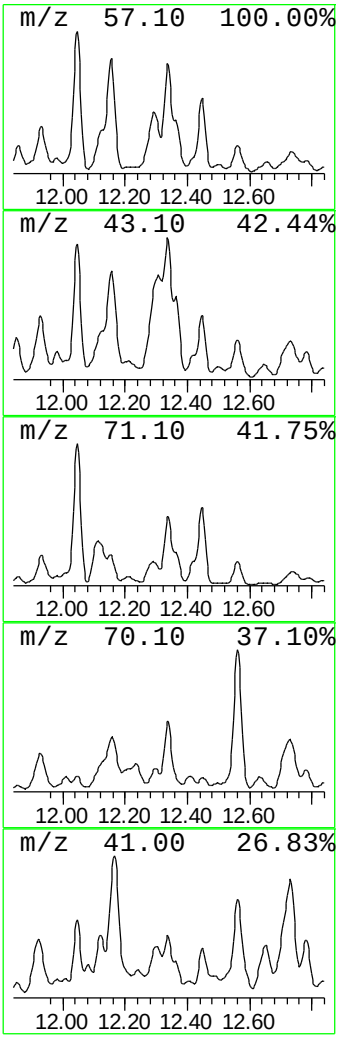
Peak Number 10 Nonane, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.34	278.91 ug/l	9526130	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonane, 4-methyl-	142	C10H22	017301-94-9	64
2	Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	53
3	Octane, 2,5-dimethyl-	142	C10H22	015869-89-3	50
4	Heptane, 2,3,4-trimethyl-	142	C10H22	052896-95-4	50
5	Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	43





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN050219\
Data File : VN055353.D
Acq On : 2 May 2019 16:44
Operator : JC/SP
Sample : K2658-09 5X
Misc : 5.65g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : EP1-SB-E2-3(14-17)

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, ethyl-	10.95	132.2	ug/l	4516640	3	11.41	1707750	50.0
Cyclohexane, 1,1,...	11.00	203.1	ug/l	6937160	3	11.41	1707750	50.0
unknown11.20	11.20	364.5	ug/l	12450200	3	11.41	1707750	50.0
Octane, 3-methyl-	11.30	255.6	ug/l	8730450	3	11.41	1707750	50.0
1-Ethyl-4-methylc...	11.70	184.9	ug/l	6314340	3	11.41	1707750	50.0
Nonane, 3-methyl-	12.05	213.8	ug/l	7302480	3	11.41	1707750	50.0
Pentalene, octahy...	12.12	276.6	ug/l	9447720	3	11.41	1707750	50.0
Cyclohexane, propyl-	12.17	644.3	ug/l	22004500	3	11.41	1707750	50.0
unknown12.30	12.30	134.5	ug/l	4594640	3	11.41	1707750	50.0
Nonane, 4-methyl-	12.34	278.9	ug/l	9526130	3	11.41	1707750	50.0