LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN121918\
Data File : VN053038.D
Acq On : 20 Dec 2018 4:10
Operator : MD\SY
Sample : J6411-06 10X
Misc : 5.07g/5.0mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 45 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : EP1-MW-K(12-13FT)1218

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\82N121818W.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	1789	1809	1820	rBV	684373	1715663	3.04%	0.288%
2	7.667	1820	1833	1851	rVB	1576195	3707554	6.57%	0.622%
3	8.027	1926	1945	1966	rBV	788930	1837884	3.26%	0.308%
4	8.587	2100	2119	2146	rBV	2247982	4628286	8.21%	0.777%
5	9.870	2497	2518	2540	rVB2	292435	783254	1.39%	0.131%
6	10.091	2573	2587	2610	rVB	3689366	6869919	12.18%	1.153%
7	10.432	2685	2693	2710	rVB	793407	1491800	2.65%	0.250%
8	10.532	2710	2724	2732	rBV2	408840	888546	1.58%	0.149%
9	10.625	2745	2753	2763	rVB	652125	1034503	1.83%	0.174%
10	10.718	2763	2782	2795	rVB	3116143	5257261	9.32%	0.882%
11	10.821	2796	2814	2827	rBV	1645430	3733028	6.62%	0.627%
12	10.889	2827	2835	2841	rBV2	606026	1016586	1.80%	0.171%
13	11.008	2857	2872	2882	rBV2	5745755	11335437	20.10%	1.903%
14	11.059	2882	2888	2895	rVV	996932	1577386	2.80%	0.265%
15	11.124	2896	2908	2916	rVV5	3745717	7185717	12.74%	1.206%
16	11.198	2916	2931	2951	rVB4	5405975	16282153	28.87%	2.733%
17	11.300	2951	2963	2972	rBV	5479978	9328692	16.54%	1.566%
18	11.406	2986	2996	3005	rBV	2985377	5227652	9.27%	0.877%
19	11.493	3016	3023	3030	rBV3	404284	678666	1.20%	0.114%
20	11.542	3030	3038	3045	rVV	2298602	3643935	6.46%	0.612%
21	11.593	3045	3054	3064	rVV7	3932095	8601961	15.25%	1.444%
22	11.654	3064	3073	3081	rVV2	8222906	15800087	28.02%	2.652%
23	11.699	3082	3087	3097	rVB2	6355046	9771476	17.33%	1.640%
24	11.760	3097	3106	3113	rBV3	1630596	3019281	5.35%	0.507%
25	11.853	3128	3135	3143	rVB4	2487935	3753174	6.65%	0.630%
26	11.924	3143	3157	3169	rBV5	11005436	27036896	47.94%	4.538%
27	12.046	3187	3195	3203	rBV	15616873	21558114	38.22%	3.618%
28	12.120	3210	3218	3223	rBV3	7291425	11885963	21.08%	1.995%
29	12.162	3224	3231	3242	rVB5	14474628	26276281	46.59%	4.410%
30	12.246	3252	3257	3264	rBV3	2857144	3757448	6.66%	0.631%
31	12.297	3267	3273	3280	rVV6	6052367	11277724	20.00%	1.893%
32	12.336	3281	3285	3296	rVB	13264583	19254553	34.14%	3.232%
33	12.403	3296	3306	3316	rBV6	4951634	9993826	17.72%	1.677%
34	12.490	3317	3333	3339	rBV7	3395464	9652215	17.11%	1.620%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN121918\
Data File : VN053038.D
Acq On : 20 Dec 2018 4:10
Operator : MD\SY
Sample : J6411-06 10X
Misc : 5.07g/5.0mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 45 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : EP1-MW-K(12-13FT)1218

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\82N121818W.M
Title : SW846 8260

35	12.564	3348	3356	3369	rVB3	17633473	33493362	59.39%	5.622%
36	12.648	3370	3382	3390	rBV5	7419037	17040020	30.21%	2.860%
37	12.728	3393	3407	3416	rVV6	19786586	56398259	100.00%	9.466%
38	12.779	3418	3423	3434	rVB3	11338659	18049023	32.00%	3.029%
39	12.869	3444	3451	3458	rBV3	5206017	7186880	12.74%	1.206%
40	12.908	3459	3463	3466	rBV2	2169605	2383220	4.23%	0.400%
41	12.963	3473	3480	3494	rVB3	17793394	31007706	54.98%	5.204%
42	13.043	3496	3505	3513	rBV4	7049738	12508415	22.18%	2.099%
43	13.168	3532	3544	3552	rVB7	7159492	15060021	26.70%	2.528%
44	13.242	3553	3567	3575	rBV2	15682737	32127665	56.97%	5.392%
45	13.596	3669	3677	3688	rBV2	4104884	8669769	15.37%	1.455%
46	13.664	3689	3698	3708	rVV5	13646689	25907436	45.94%	4.348%
47	13.712	3709	3713	3721	rVB3	3094201	3988921	7.07%	0.670%
48	13.889	3761	3768	3778	rVB	10172545	15873097	28.14%	2.664%
49	13.995	3792	3801	3812	rVB5	5662730	10560006	18.72%	1.772%
50	14.175	3848	3857	3864	rBV4	4773625	9489692	16.83%	1.593%
51	14.249	3874	3880	3888	rVB	5564734	7823315	13.87%	1.313%
52	14.294	3888	3894	3900	rBV3	1726657	2141185	3.80%	0.359%
53	14.332	3900	3906	3913	rVV2	1997114	2454531	4.35%	0.412%
54	14.480	3944	3952	3960	rBV5	1142465	2718561	4.82%	0.456%
55	14.525	3961	3966	3974	rVB2	2156040	3023757	5.36%	0.508%
56	14.580	3975	3983	3996	rVB2	1594521	2855097	5.06%	0.479%
57	14.648	3997	4004	4015	rVB2	1320463	2188445	3.88%	0.367%
58	14.850	4062	4067	4073	rBV4	477088	577724	1.02%	0.097%
59	14.956	4092	4100	4111	rVB4	900344	1838992	3.26%	0.309%
60	15.239	4181	4188	4210	rVB7	209367	568812	1.01%	0.095%

Sum of corrected areas: 595796832

LSC Report - Integrated Chromatogram

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN121918\
Data File : VN053038.D
Acq On : 20 Dec 2018 4:10
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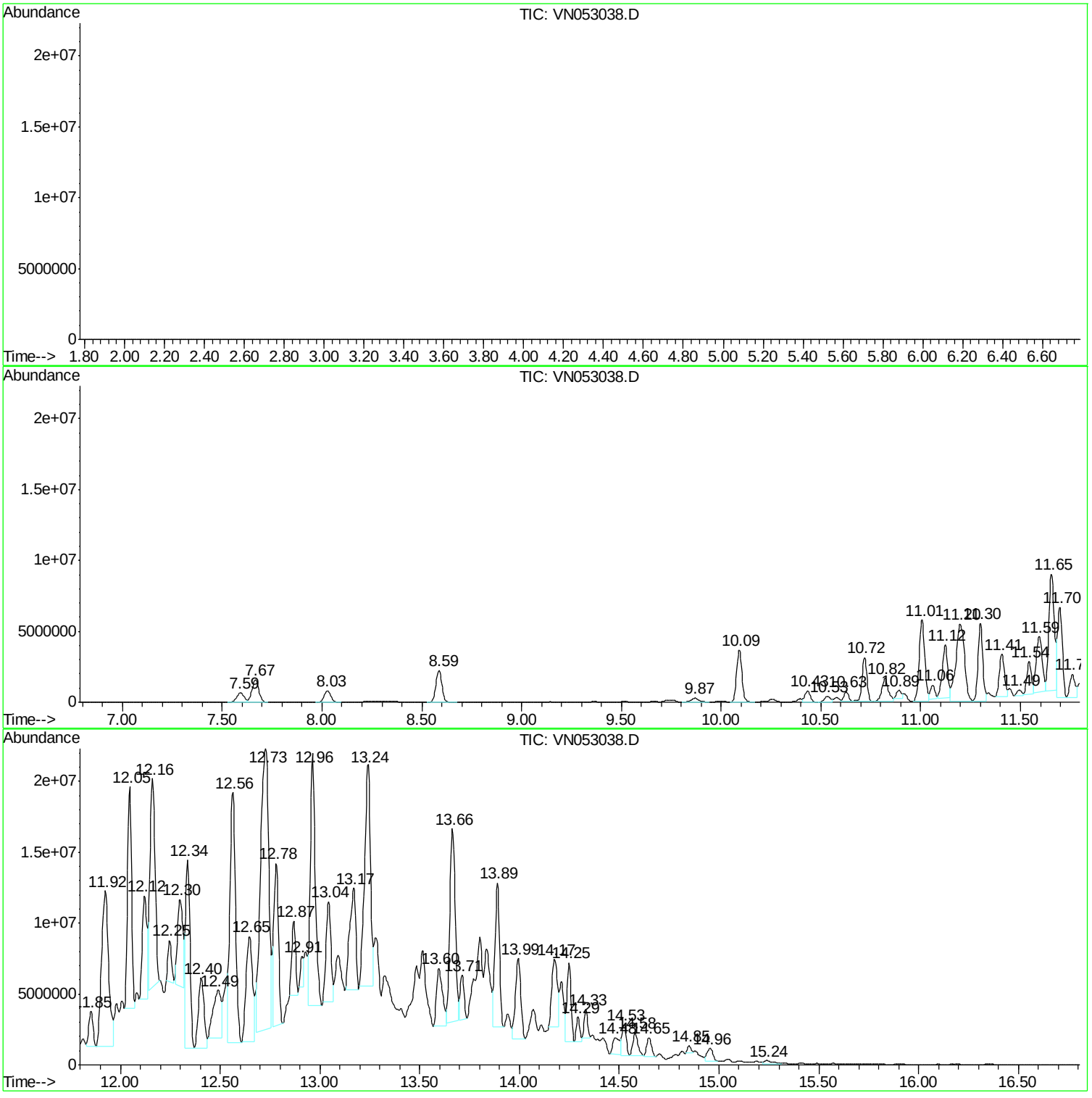
Sample : J6411-06 10X
Misc : 5.07g/5.0mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 45 Sample Multiplier: 28

Instrument :
MSVOA_N
ClientSampleId :
EP1-MW-K(12-13FT)1218

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N121818W.M
Quant Title : SW846 8260

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



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN121918\
Data File : VN053038.D
Acq On : 20 Dec 2018 4:10
Operator : MD\SY
Sample : J6411-06 10X
Misc : 5.07g/5.0mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 45 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : EP1-MW-K(12-13FT)1218

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N121818W.M
Quant Title : SW846 8260

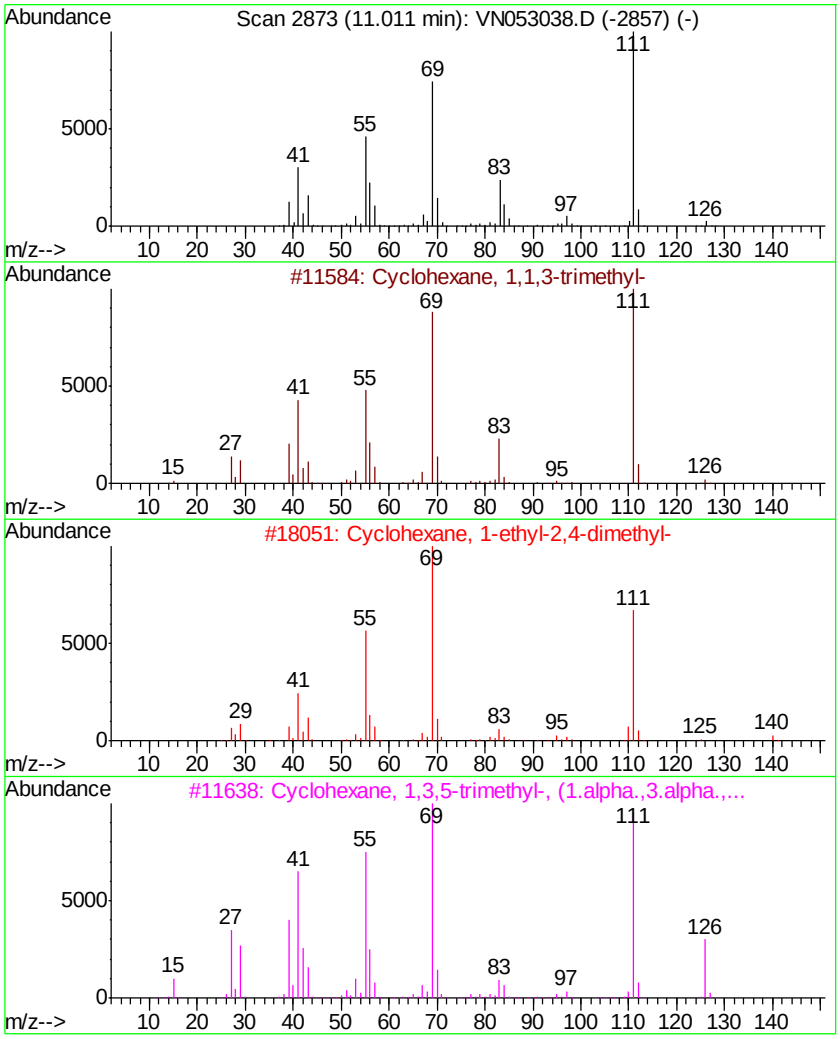
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

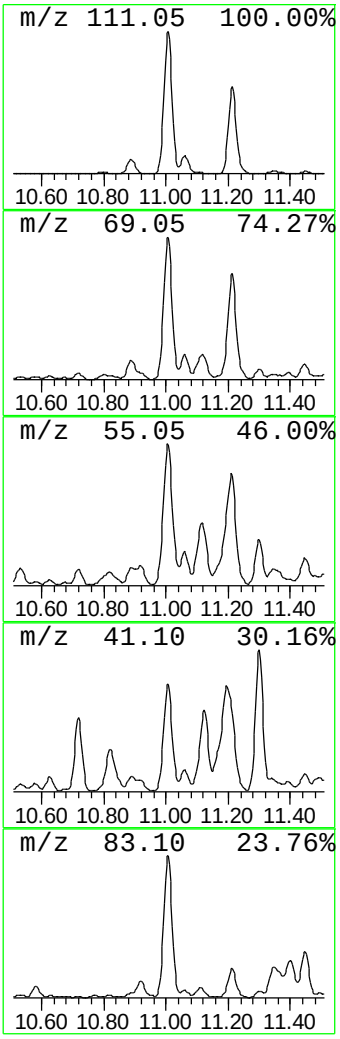
****

Peak Number 1 Cyclohexane, 1,1,3-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.01	108.42 ug/l	11335400	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,1,3-trimethyl-	126	C9H18	003073-66-3	94
2	Cyclohexane, 1-ethyl-2,4-dimethyl-	140	C10H20	061142-69-6	64
3	Cyclohexane, 1,3,5-trimethyl-, (...	126	C9H18	001795-26-2	64
4	Cyclooctane, (1-methylpropyl)-	168	C12H24	016538-89-9	64
5	Cyclohexane, 1,2,4-trimethyl-, (...	126	C9H18	007667-60-9	53





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN121918\
Data File : VN053038.D
Acq On : 20 Dec 2018 4:10
Operator : MD\SY
Sample : J6411-06 10X
Misc : 5.07g/5.0mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 45 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : EP1-MW-K(12-13FT)1218

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N121818W.M
Quant Title : SW846 8260

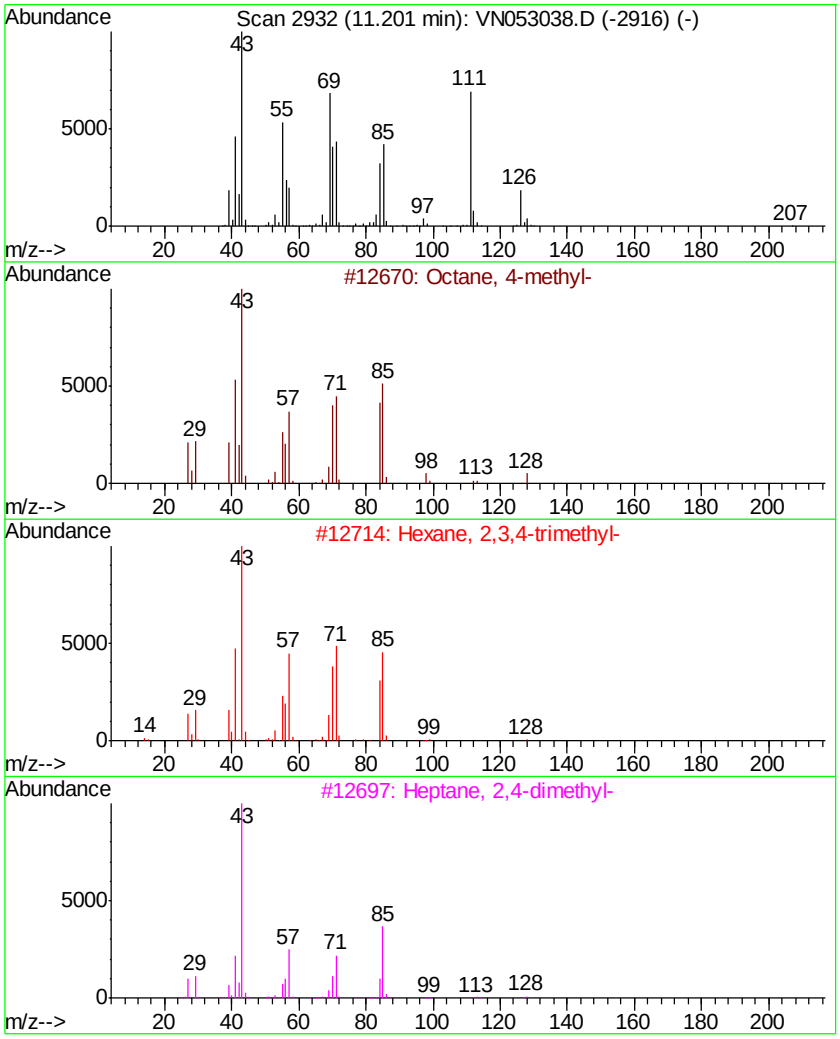
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

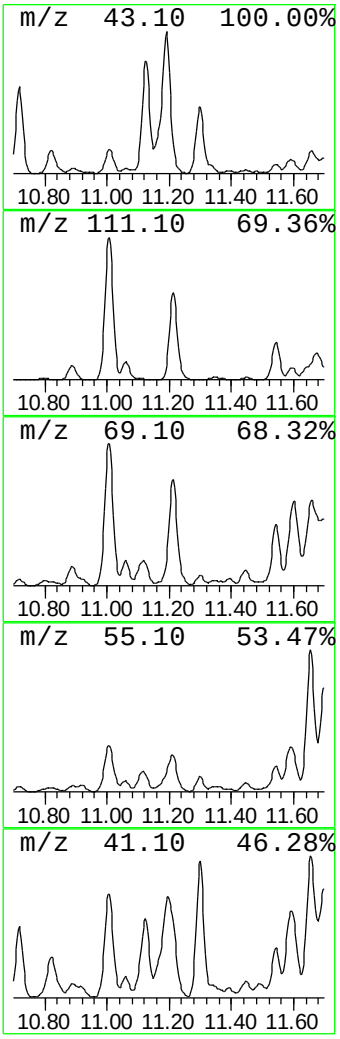
****

Peak Number 2 Octane, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.20	155.73 ug/l	16282200	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 4-methyl-	128	C9H20	002216-34-4	83
2	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	53
3	Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	43
4	Hexane, 3-ethyl-	114	C8H18	000619-99-8	43
5	Hexane, 2,3,5-trimethyl-	128	C9H20	001069-53-0	41





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN121918\
Data File : VN053038.D
Acq On : 20 Dec 2018 4:10
Operator : MD\SY
Sample : J6411-06 10X
Misc : 5.07g/5.0mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 45 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : EP1-MW-K(12-13FT)1218

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N121818W.M
Quant Title : SW846 8260

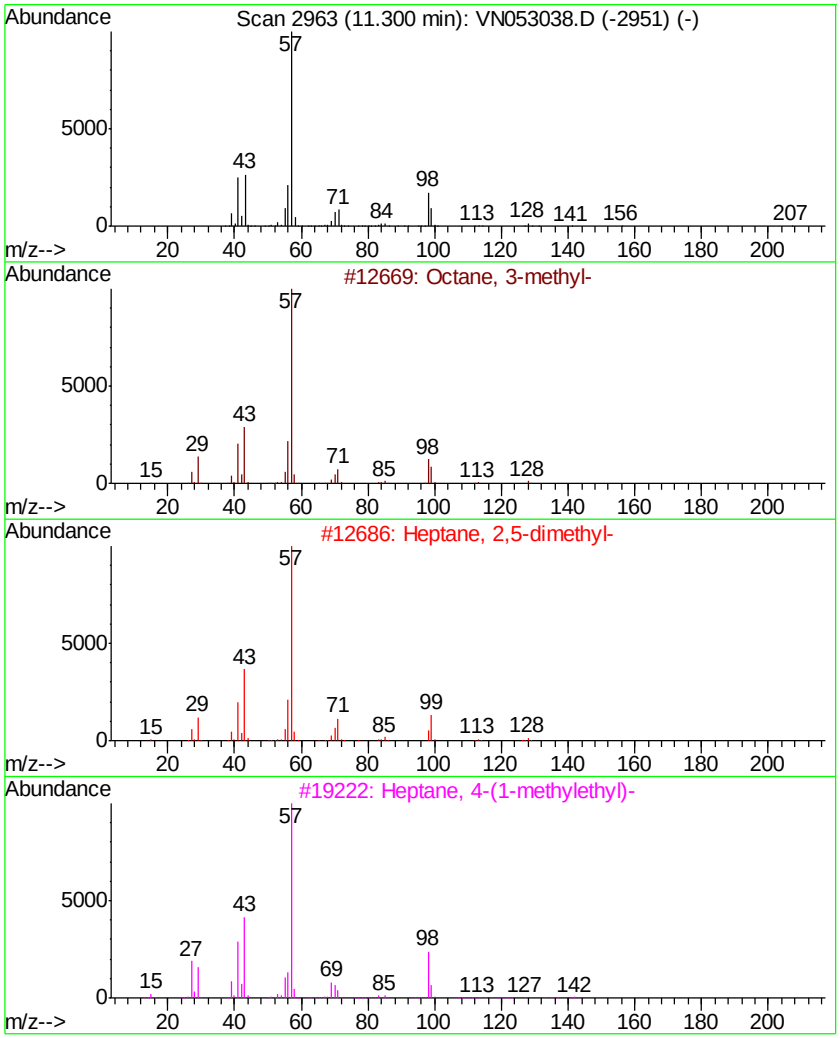
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

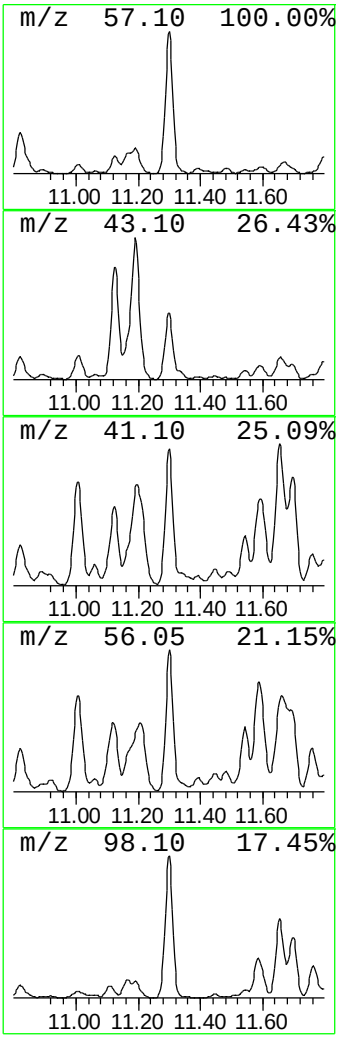
****

Peak Number 3 Octane, 3-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.30	89.22 ug/l	9328690	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	90
3	Heptane, 4-(1-methylethyl)-	142	C10H22	052896-87-4	64
4	Heptane, 3,5-dimethyl-	128	C9H20	000926-82-9	59
5	Undecane, 6-methyl-	170	C12H26	017302-33-9	59





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN121918\
Data File : VN053038.D
Acq On : 20 Dec 2018 4:10
Operator : MD\SY
Sample : J6411-06 10X
Misc : 5.07g/5.0mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 45 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : EP1-MW-K(12-13FT)1218

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N121818W.M
Quant Title : SW846 8260

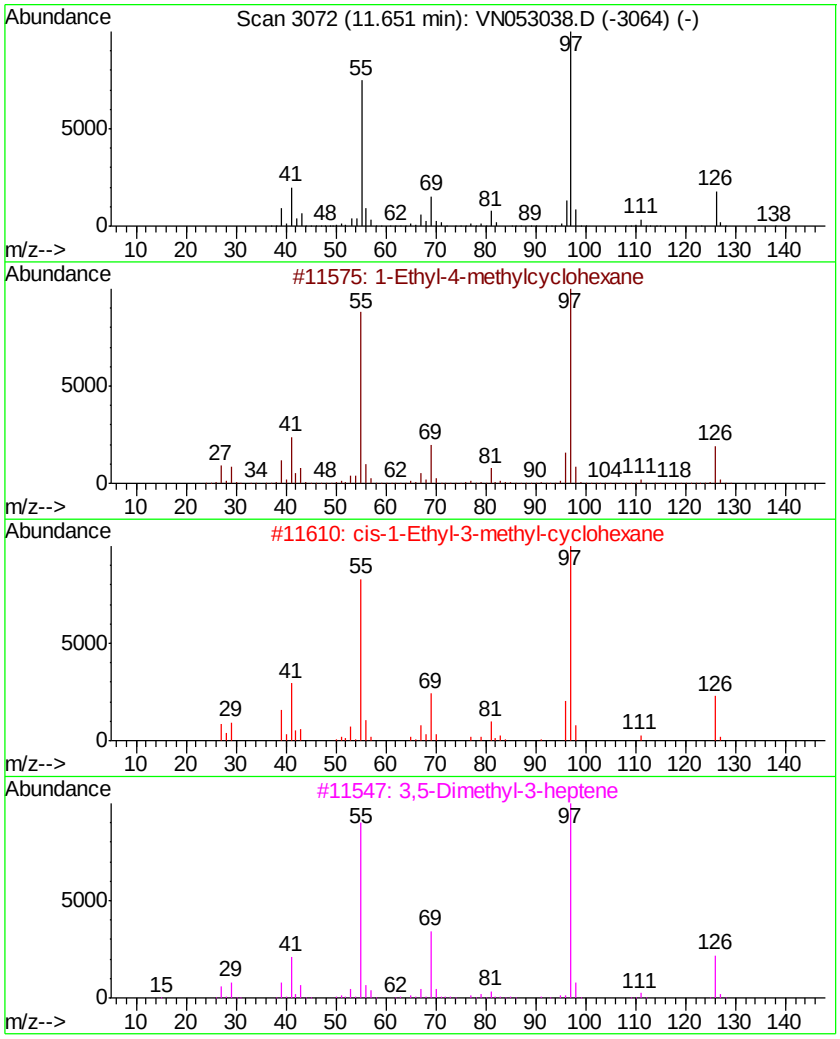
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

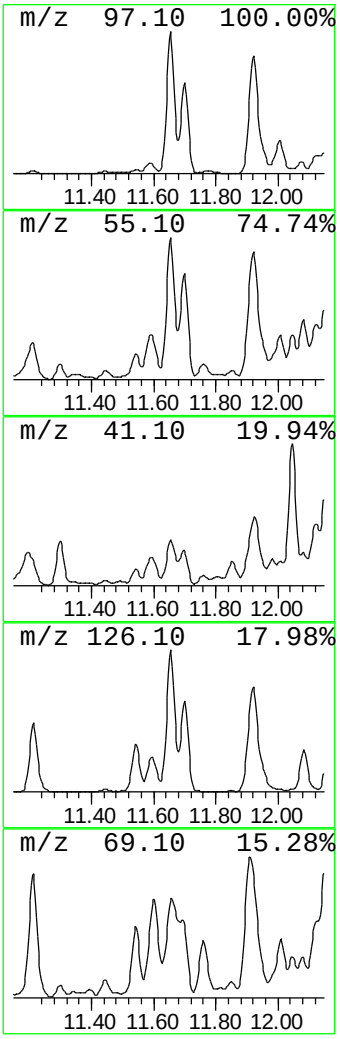
****

Peak Number 4 1-Ethyl-4-methylcyclohexane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.65	151.12 ug/l	15800100	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Ethyl-4-methylcyclohexane	126	C9H18	003728-56-1	95
2	cis-1-Ethyl-3-methyl-cyclohexane	126	C9H18	019489-10-2	87
3	3,5-Dimethyl-3-heptene	126	C9H18	059643-68-4	87
4	Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	004926-78-7	78
5	4-Octen-3-one	126	C8H14O	014129-48-7	72





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN121918\
Data File : VN053038.D
Acq On : 20 Dec 2018 4:10
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Misc : 5.07g/5.0mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 45 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : EP1-MW-K(12-13FT)1218

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N121818W.M
Quant Title : SW846 8260

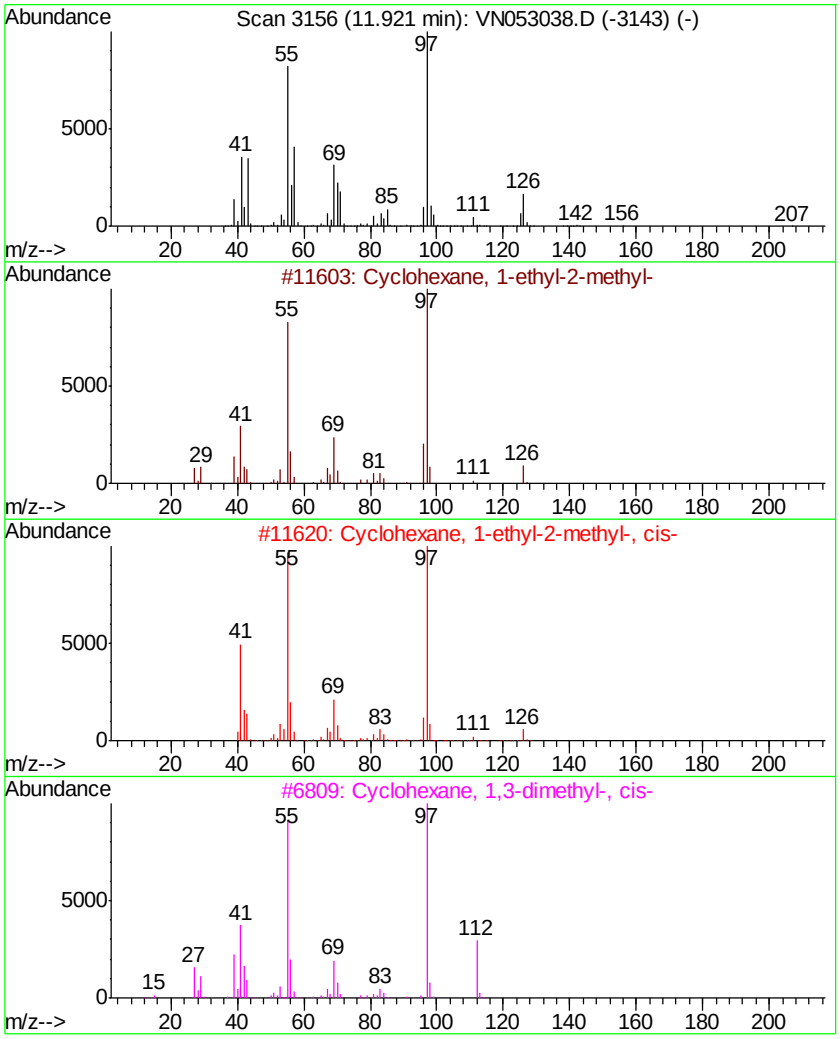
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

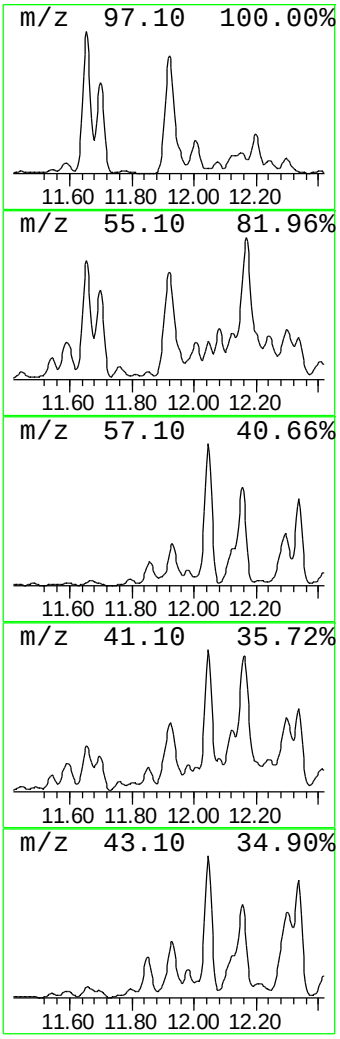
****

Peak Number 6 Cyclohexane, 1-ethyl-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	258.60 ug/l	27036900	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1-ethyl-2-methyl-	126	C9H18	003728-54-9	58
2	Cyclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-77-7	53
3	Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	53
4	2-Hexene, 3,4,4-trimethyl-	126	C9H18	053941-19-8	52
5	Cyclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-78-8	52





Library Search Compound Report

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Operator : MD\SY
Sample : J6411-06 10X
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ALS Vial : 45 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : EP1-MW-K(12-13FT)1218

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N121818W.M
Quant Title : SW846 8260

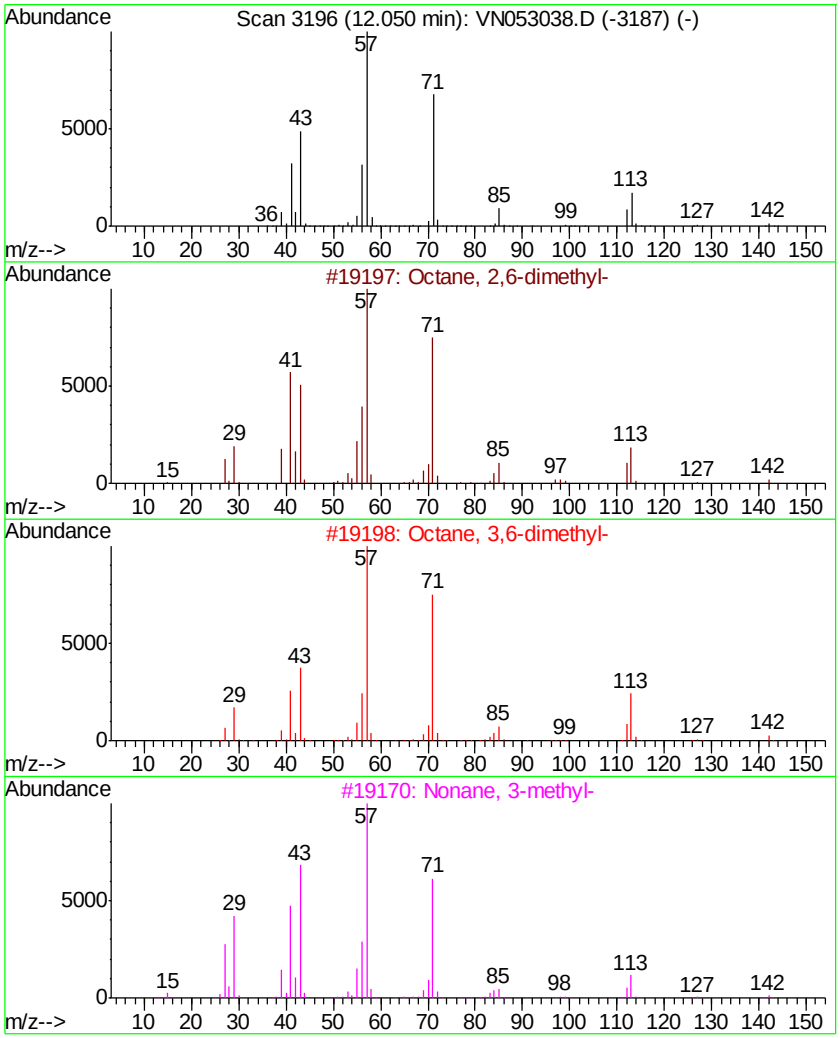
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

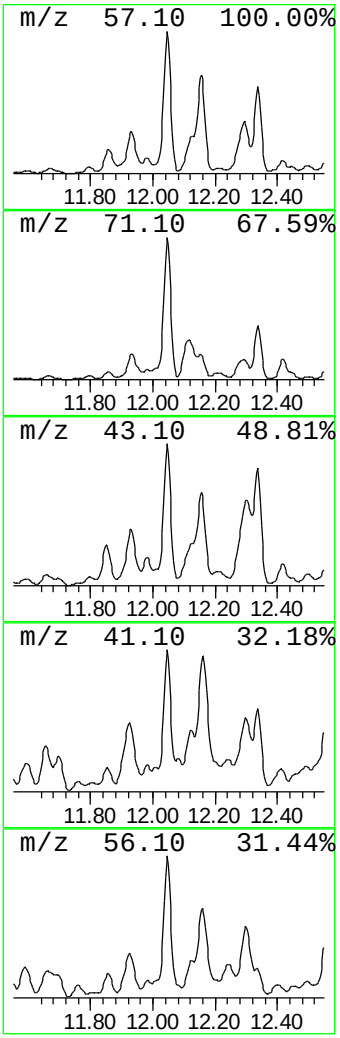
****

Peak Number 7 Octane, 2,6-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.05	206.19 ug/l	21558100	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	91
4	Undecane, 6,6-dimethyl-	184	C13H28	017312-76-4	64
5	Sulfurous acid, 2-ethylhexyl hex...	418	C24H50O3S	1000309-19-9	64





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN121918\
Data File : VN053038.D
Acq On : 20 Dec 2018 4:10
Operator : MD\SY
Sample : J6411-06 10X
Misc : 5.07g/5.0mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 45 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : EP1-MW-K(12-13FT)1218

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N121818W.M
Quant Title : SW846 8260

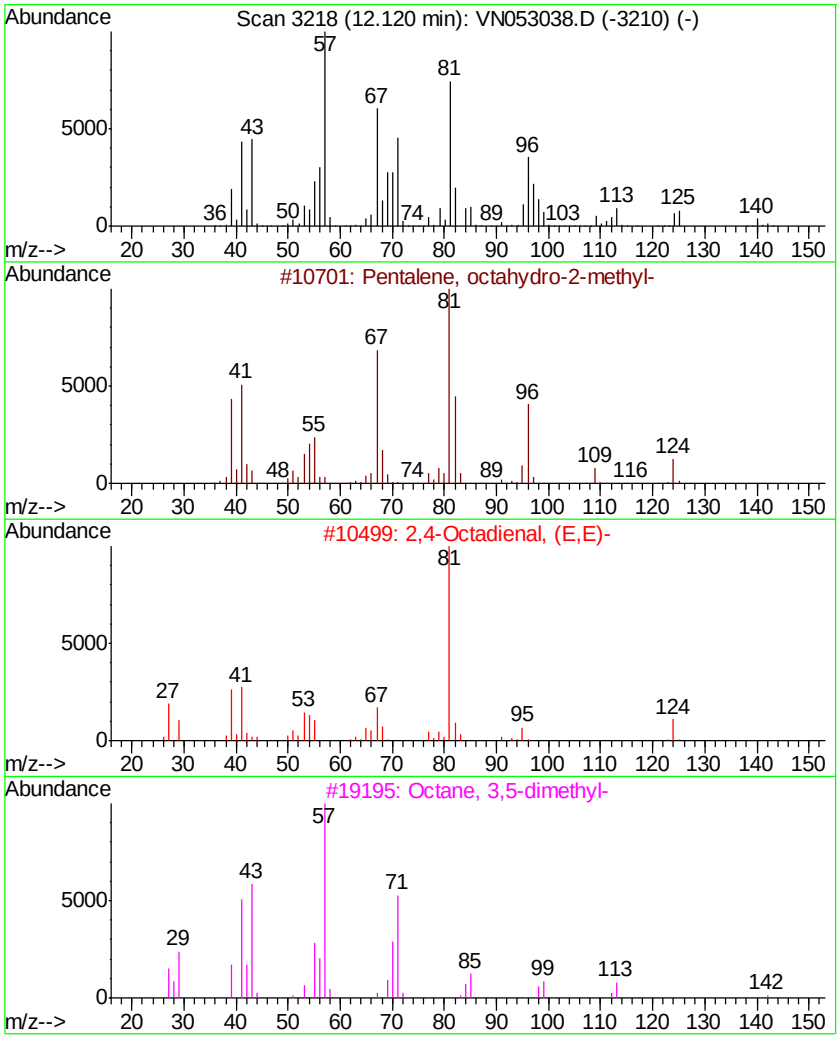
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

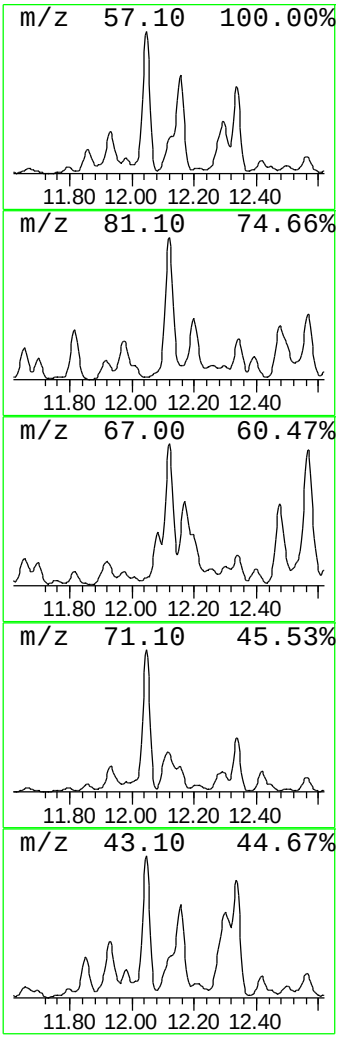
****

Peak Number 8 Pentalene, octahydro-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.12	113.68 ug/l	11886000	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentalene, octahydro-2-methyl-	124	C9H16	003868-64-2	60
2	2,4-Octadienal, (E,E)-	124	C8H12O	030361-28-5	25
3	Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	20
4	1H-Indene, octahydro-, trans-	124	C9H16	003296-50-2	18
5	Cyclopentane, ethylidene-	96	C7H12	002146-37-4	18





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN121918\
Data File : VN053038.D
Acq On : 20 Dec 2018 4:10
Operator : MD\SY
Sample : J6411-06 10X
Misc : 5.07g/5.0mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 45 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : EP1-MW-K(12-13FT)1218

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N121818W.M
Quant Title : SW846 8260

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

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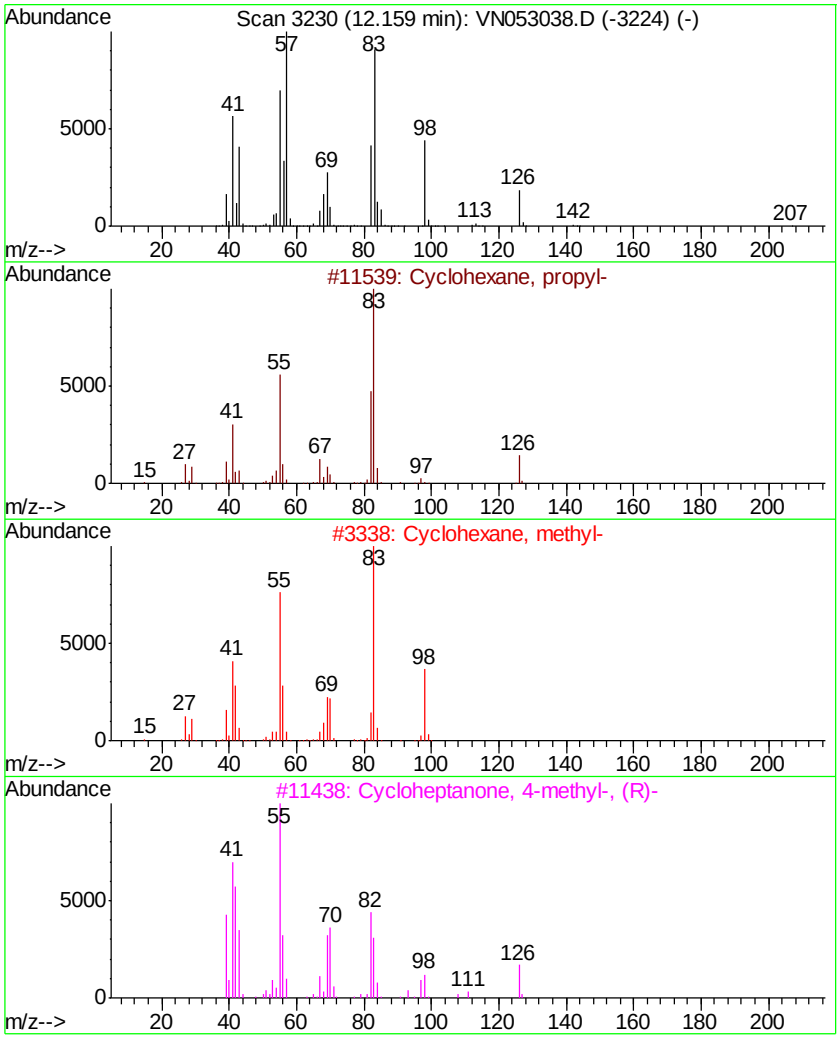
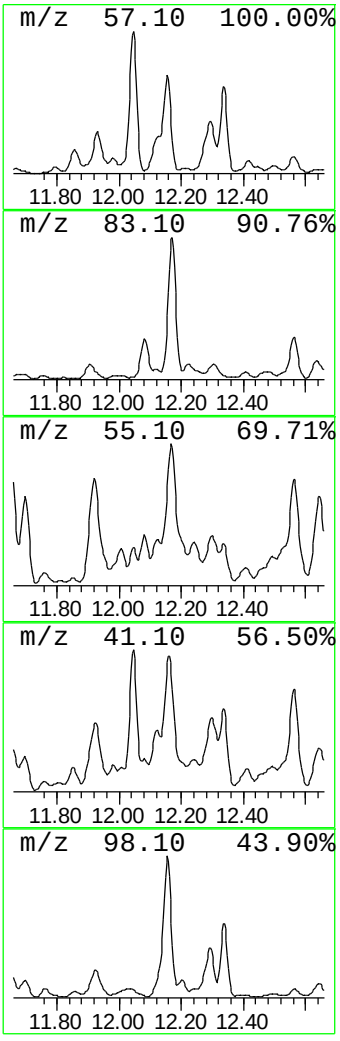
Peak Number 9 Cyclohexane, propyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.16	251.32 ug/l	26276300	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, propyl-	126	C9H18	001678-92-8	62
2	Cyclohexane, methyl-	98	C7H14	000108-87-2	58
3	Cycloheptanone, 4-methyl-, (R)-	126	C8H14O	013609-59-1	46
4	2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	46
5	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	43





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN121918\
Data File : VN053038.D
Acq On : 20 Dec 2018 4:10
Operator : MD\SY
Sample : J6411-06 10X
Misc : 5.07g/5.0mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 45 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : EP1-MW-K(12-13FT)1218

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N121818W.M
Quant Title : SW846 8260

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

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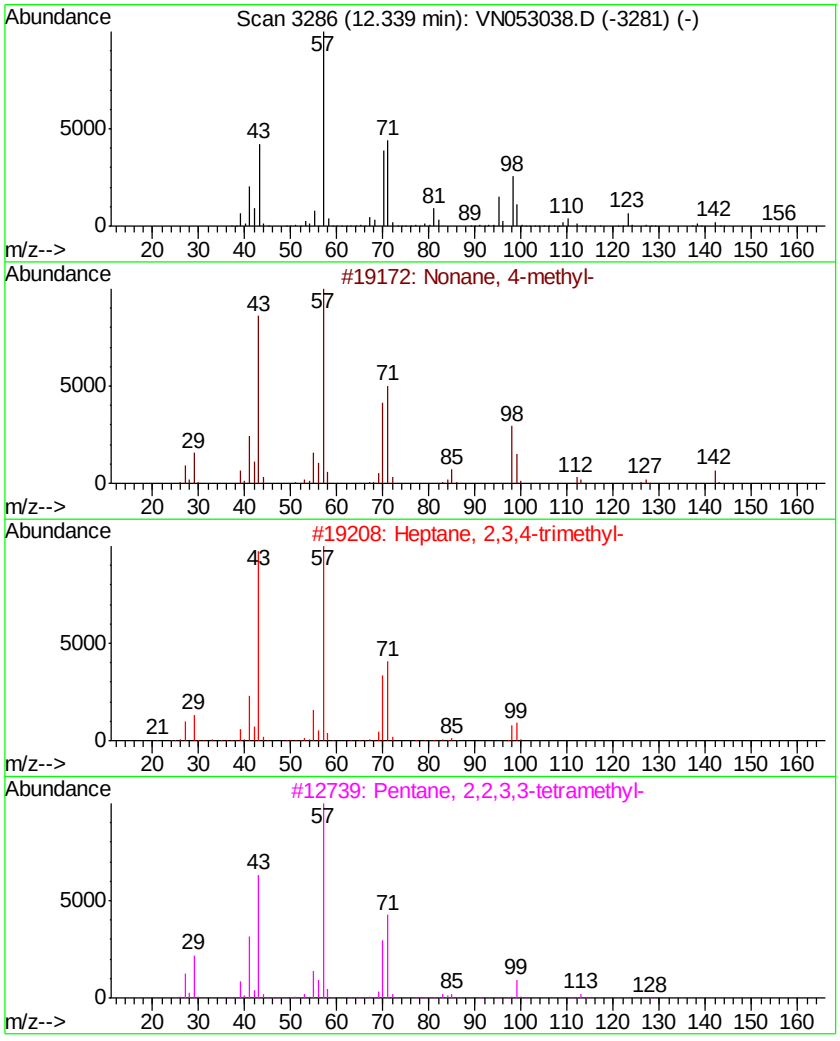
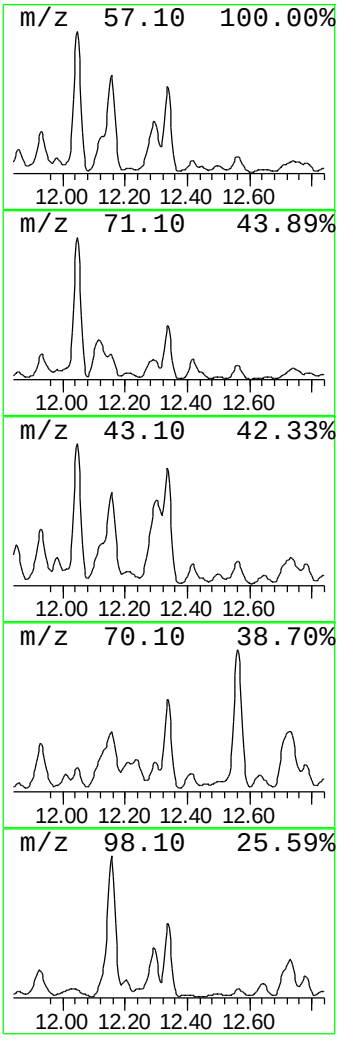
Peak Number 10 Nonane, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.34	184.16 ug/l	19254600	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonane, 4-methyl-	142	C10H22	017301-94-9	72
2	Heptane, 2,3,4-trimethyl-	142	C10H22	052896-95-4	59
3	Pentane, 2,2,3,3-tetramethyl-	128	C9H20	007154-79-2	53
4	Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	43
5	Decane, 2,5,9-trimethyl-	184	C13H28	062108-22-9	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN121918\
Data File : VN053038.D
Acq On : 20 Dec 2018 4:10
Operator : MD\SY
Sample : J6411-06 10X
Misc : 5.07g/5.0mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 45 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : EP1-MW-K(12-13FT)1218

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N121818W.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,...	11.01	108.4	ug/l	11335400	3	11.41	5227650	50.0
Octane, 4-methyl-	11.20	155.7	ug/l	16282200	3	11.41	5227650	50.0
Octane, 3-methyl-	11.30	89.2	ug/l	9328690	3	11.41	5227650	50.0
1-Ethyl-4-methylc...	11.65	151.1	ug/l	15800100	3	11.41	5227650	50.0
Cyclohexane, 1-et...	11.92	258.6	ug/l	27036900	3	11.41	5227650	50.0
Octane, 2,6-dimet...	12.05	206.2	ug/l	21558100	3	11.41	5227650	50.0
Pentalene, octahy...	12.12	113.7	ug/l	11886000	3	11.41	5227650	50.0
Cyclohexane, propyl-	12.16	251.3	ug/l	26276300	3	11.41	5227650	50.0
Nonane, 4-methyl-	12.34	184.2	ug/l	19254600	3	11.41	5227650	50.0