LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN121918\
Data File : VN053035.D
Acq On : 20 Dec 2018 2:50
Operator : MD\SY
Sample : J6411-11 10X
Misc : 5.24g/5.0mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 42 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : EP1-SBR-4A(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	1785	1809	1820	rBV	669283	1666598	3.29%	0.337%
2	7.667	1820	1833	1854	rVB	1495603	3529810	6.97%	0.714%
3	8.027	1926	1945	1969	rBV	768311	1777781	3.51%	0.359%
4	8.587	2102	2119	2140	rBV	2144039	4419217	8.72%	0.893%
5	10.091	2572	2587	2615	rVB	3842296	7226630	14.26%	1.461%
6	10.432	2685	2693	2709	rVB	334519	622676	1.23%	0.126%
7	10.718	2771	2782	2793	rVB	907642	1512678	2.99%	0.306%
8	10.818	2794	2813	2826	rBV	578706	1285495	2.54%	0.260%
9	10.886	2826	2834	2842	rBV3	317215	549040	1.08%	0.111%
10	10.953	2846	2855	2862	rVV	1135727	1743802	3.44%	0.352%
11	11.005	2862	2871	2882	rVB2	1951996	3370083	6.65%	0.681%
12	11.124	2896	2908	2916	rBV3	1394097	2573631	5.08%	0.520%
13	11.201	2916	2932	2951	rVB7	2505312	7227610	14.26%	1.461%
14	11.300	2951	2963	2983	rBV	3415428	6173040	12.18%	1.248%
15	11.407	2984	2996	3014	rBV	3068588	5799811	11.44%	1.172%
16	11.490	3015	3022	3030	rBV4	284582	520988	1.03%	0.105%
17	11.542	3030	3038	3045	rBV	1006306	1547386	3.05%	0.313%
18	11.596	3045	3055	3063	rBV7	1637586	3250111	6.41%	0.657%
19	11.654	3064	3073	3081	rVV2	4688912	8445537	16.67%	1.707%
20	11.696	3081	3086	3097	rVB2	3312295	5395655	10.65%	1.091%
21	11.760	3097	3106	3111	rBV3	988623	1733326	3.42%	0.350%
22	11.853	3127	3135	3143	rVB3	2331918	3509228	6.92%	0.709%
23	11.924	3143	3157	3169	rBV5	7767776	18579663	36.66%	3.756%
24	11.979	3171	3174	3179	rVV2	698075	725590	1.43%	0.147%
25	12.046	3187	3195	3203	rVB	11240189	15216045	30.03%	3.076%
26	12.120	3210	3218	3223	rBV5	6075146	9983497	19.70%	2.018%
27	12.162	3224	3231	3249	rVB5	12315825	23558142	46.49%	4.762%
28	12.297	3266	3273	3279	rBV8	4444177	8135696	16.05%	1.645%
29	12.336	3280	3285	3298	rVB	10522225	17056984	33.66%	3.448%
30	12.406	3299	3307	3314	rBV6	3291863	5478707	10.81%	1.107%
31	12.448	3314	3320	3327	rBV3	3046416	4028291	7.95%	0.814%
32	12.561	3348	3355	3371	rVB4	10139833	21382724	42.20%	4.322%
33	12.654	3371	3384	3392	rBV6	9644243	20531354	40.52%	4.150%
34	12.731	3395	3408	3417	rVV5	21726174	50675909	100.00%	10.244%

LSC Area Percent Report

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Data File : VN053035.D
Acq On : 20 Dec 2018 2:50
Operator : MD\SY
Sample : J6411-11 10X
Misc : 5.24g/5.0mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 42 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : EP1-SBR-4A(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	12.779	3418	3423	3434	rVB3	7083063	11300362	22.30%	2.284%
36	12.870	3444	3451	3458	rBV5	3475007	4867718	9.61%	0.984%
37	12.927	3459	3469	3472	rVV4	2393012	4285643	8.46%	0.866%
38	12.963	3473	3480	3493	rVB3	13149513	21950785	43.32%	4.437%
39	13.040	3494	3504	3514	rBV	28566085	46717399	92.19%	9.443%
40	13.169	3533	3544	3552	rVB6	3534368	7921385	15.63%	1.601%
41	13.239	3553	3566	3574	rBV5	13086190	25205622	49.74%	5.095%
42	13.374	3601	3608	3618	rVB	11321449	17980653	35.48%	3.635%
43	13.541	3654	3660	3667	rVB	4865680	6491776	12.81%	1.312%
44	13.586	3667	3674	3689	rVB4	6366591	12165334	24.01%	2.459%
45	13.664	3689	3698	3708	rBV5	7521619	13143738	25.94%	2.657%
46	13.712	3709	3713	3721	rVB2	1997511	2471330	4.88%	0.500%
47	13.802	3736	3741	3745	rBV3	1803490	2362116	4.66%	0.477%
48	13.834	3746	3751	3760	rVV4	3686892	5644133	11.14%	1.141%
49	13.889	3761	3768	3778	rVB	5203992	8303702	16.39%	1.679%
50	13.995	3791	3801	3810	rVB3	4727465	7689478	15.17%	1.554%
51	14.050	3811	3818	3823	rBV4	1016691	1804547	3.56%	0.365%
52	14.175	3849	3857	3865	rBV5	2245200	4540230	8.96%	0.918%
53	14.249	3874	3880	3888	rVB	2828160	3960738	7.82%	0.801%
54	14.294	3888	3894	3900	rBV3	1280420	1770057	3.49%	0.358%
55	14.332	3900	3906	3914	rVB2	1854650	2521175	4.98%	0.510%
56	14.477	3945	3951	3959	rBV4	476672	960702	1.90%	0.194%
57	14.522	3961	3965	3973	rVB2	871811	1186215	2.34%	0.240%
58	14.583	3974	3984	3997	rBV2	3110253	5880255	11.60%	1.189%
59	14.648	3997	4004	4014	rVB2	561180	889589	1.76%	0.180%
60	14.741	4025	4033	4043	rVB	1764172	2614593	5.16%	0.529%
61	14.956	4092	4100	4118	rVB3	401584	842522	1.66%	0.170%

Sum of corrected areas: 494704532

LSC Report - Integrated Chromatogram

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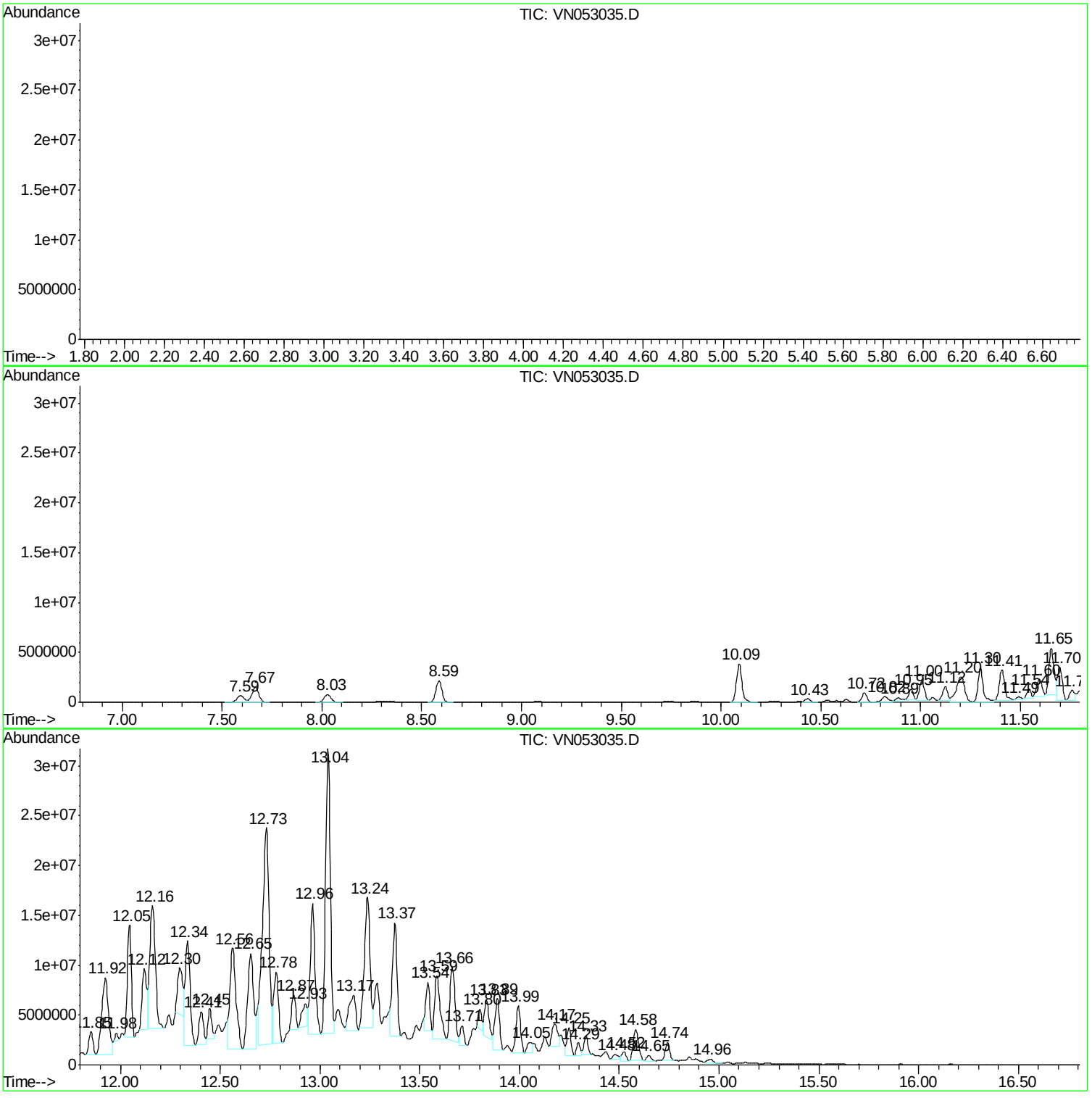
ALS Vial : 42 Sample Multiplier: 28

Instrument :
MSVOA_N
ClientSampleId :
EP1-SBR-4A(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 : VN053035.D
Acq On : 20 Dec 2018 2:50
Operator : MD\SY
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ALS Vial : 42 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : EP1-SBR-4A(12-13FT)1218

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

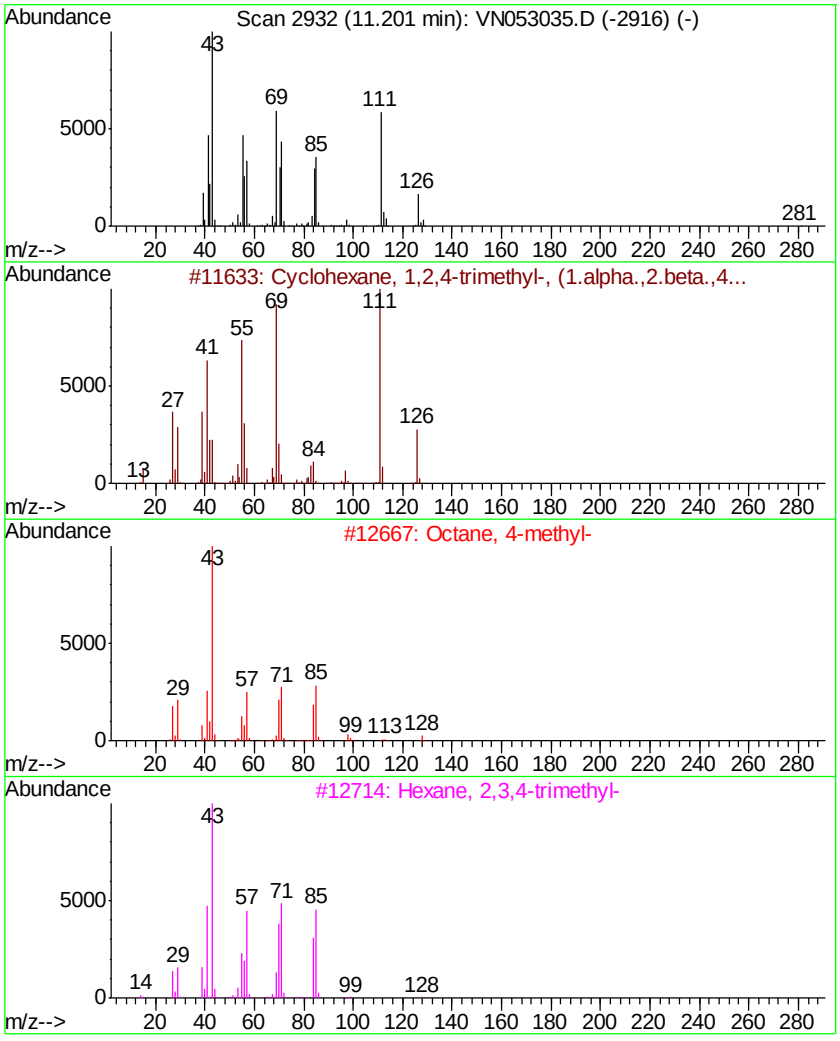
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

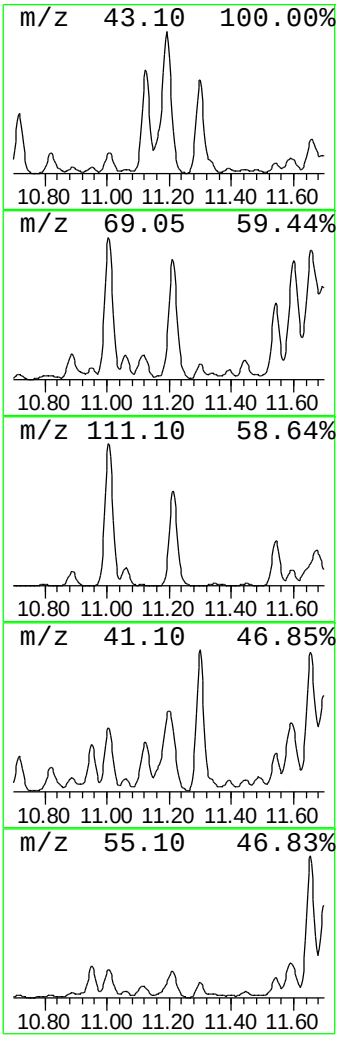
****

Peak Number 1 Cyclohexane, 1,2,4-trimethy... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.20	62.31 ug/l	7227610	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,2,4-trimethyl-, (...	126	C9H18	007667-60-9	50
2	Octane, 4-methyl-	128	C9H20	002216-34-4	49
3	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	43
4	Hexane, 3-ethyl-	114	C8H18	000619-99-8	35
5	Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	35





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN121918\
Data File : VN053035.D
Acq On : 20 Dec 2018 2:50
Operator : MD\SY
Sample : J6411-11 10X
Misc : 5.24g/5.0mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 42 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : EP1-SBR-4A(12-13FT)1218

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

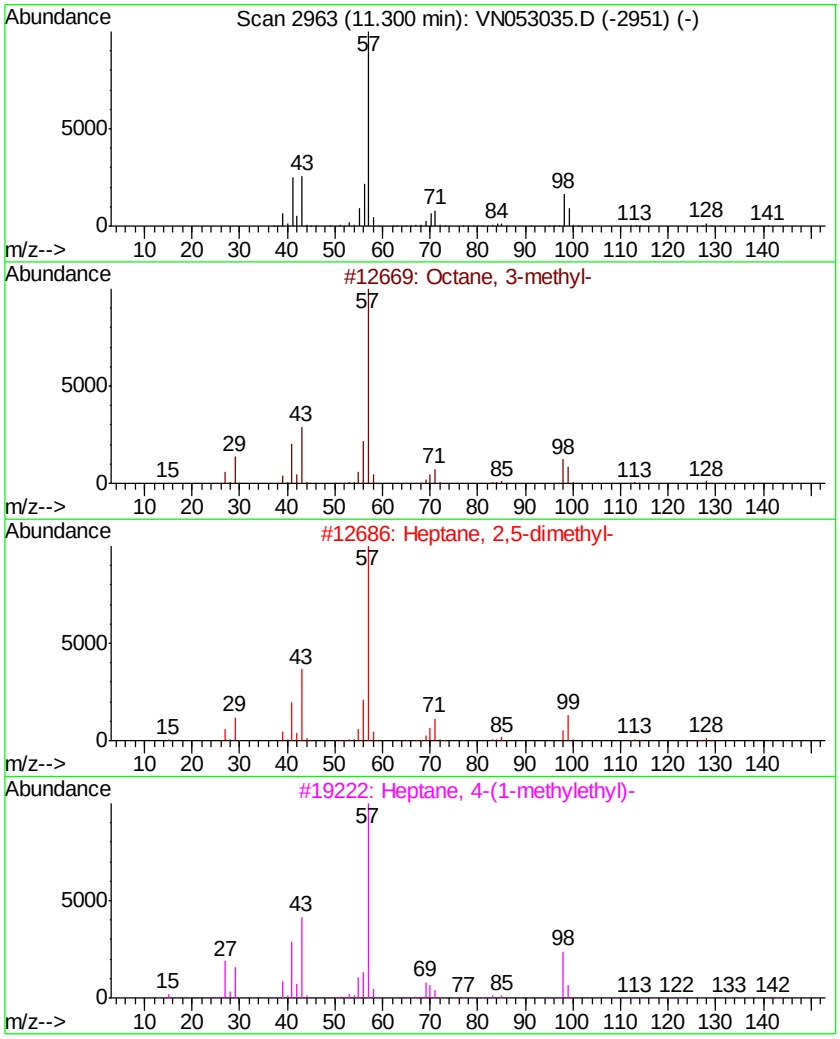
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

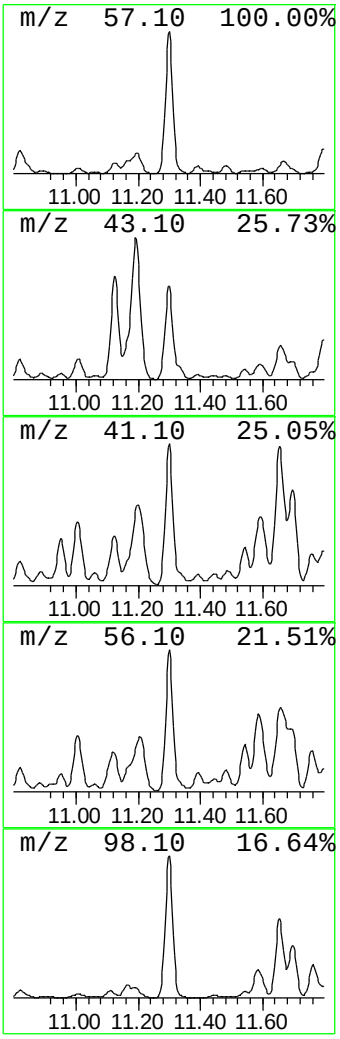
****

Peak Number 2 Octane, 3-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.30	53.22 ug/l	6173040	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	Oxalic acid, isobutyl heptyl ester	244	C13H24O4	1000309-37-2	53
5	Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	50





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Data File : VN053035.D
Acq On : 20 Dec 2018 2:50
Operator : MD\SY
Sample : J6411-11 10X
Misc : 5.24g/5.0mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 42 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : EP1-SBR-4A(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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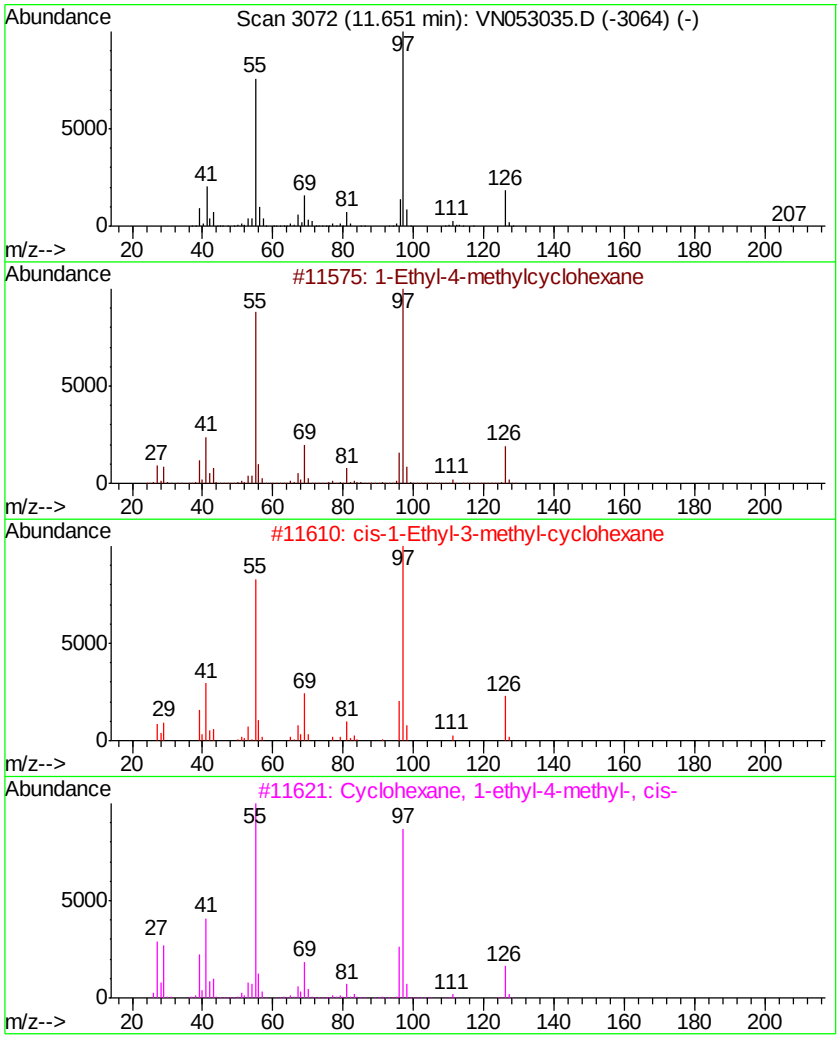
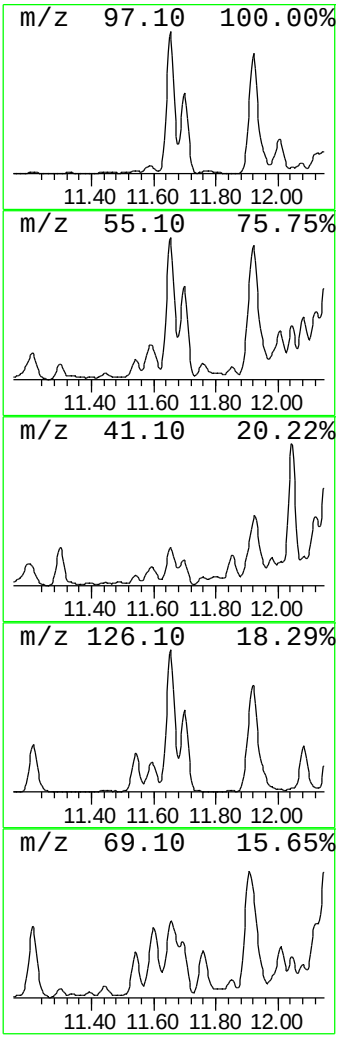
Peak Number 3 1-Ethyl-4-methylcyclohexane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.65	72.81 ug/l	8445540	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	91
3	Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	004926-78-7	87
4	3,5-Dimethyl-3-heptene	126	C9H18	059643-68-4	87
5	Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	006236-88-0	86





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ALS Vial : 42 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : EP1-SBR-4A(12-13FT)1218

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

TIC Library : C:\DATABASE\NIST11.L
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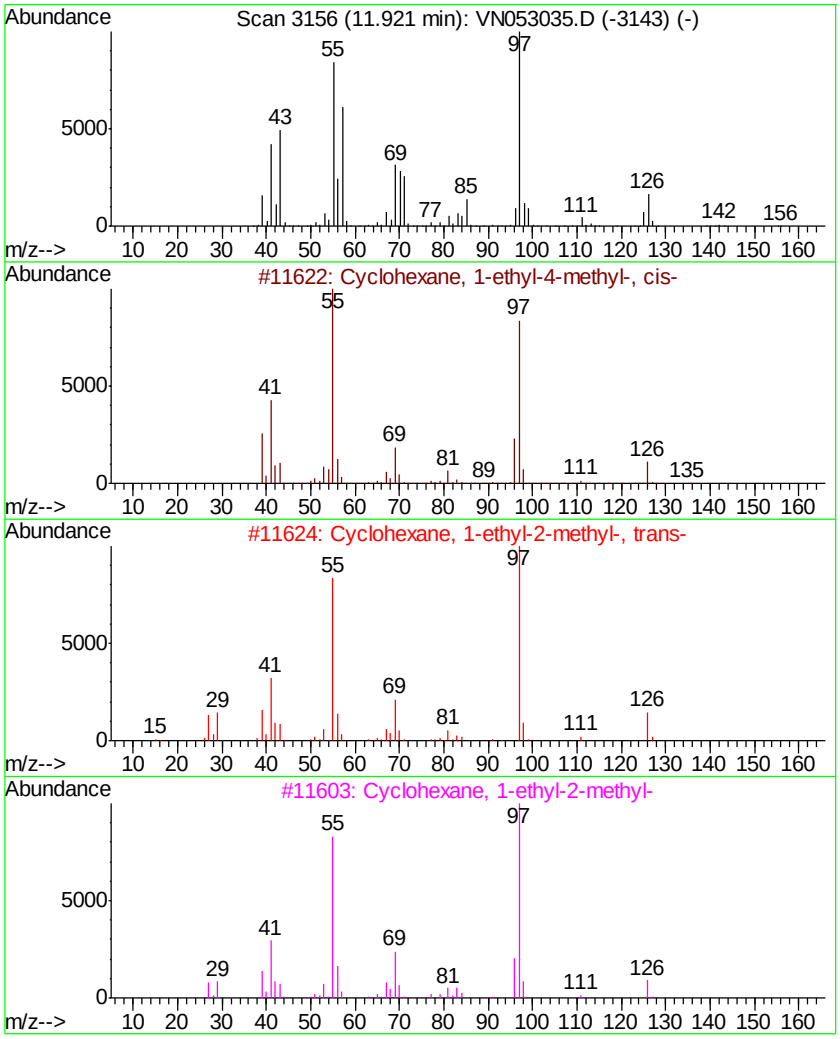
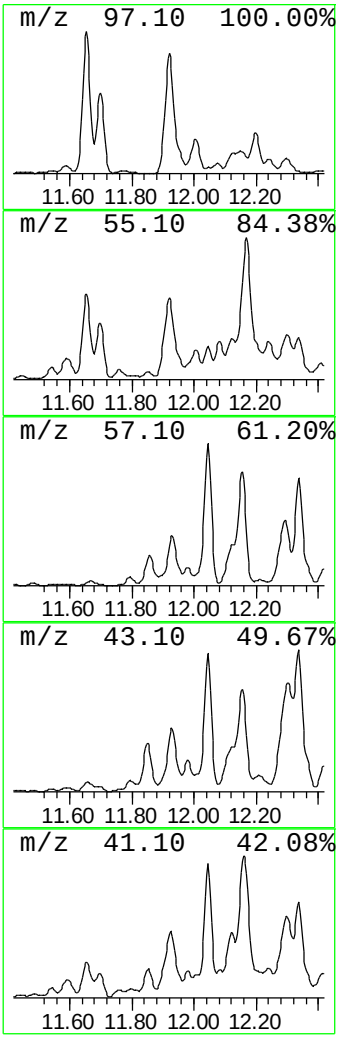
Peak Number 4 unknown11.92 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	160.18 ug/l	18579700	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	004926-78-7	49
2	Cyclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-78-8	49
3	Cyclohexane, 1-ethyl-2-methyl-	126	C9H18	003728-54-9	49
4	Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	006236-88-0	49
5	3,5-Dimethyl-3-heptene	126	C9H18	059643-68-4	43





Library Search Compound Report

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ALS Vial : 42 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : EP1-SBR-4A(12-13FT)1218

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

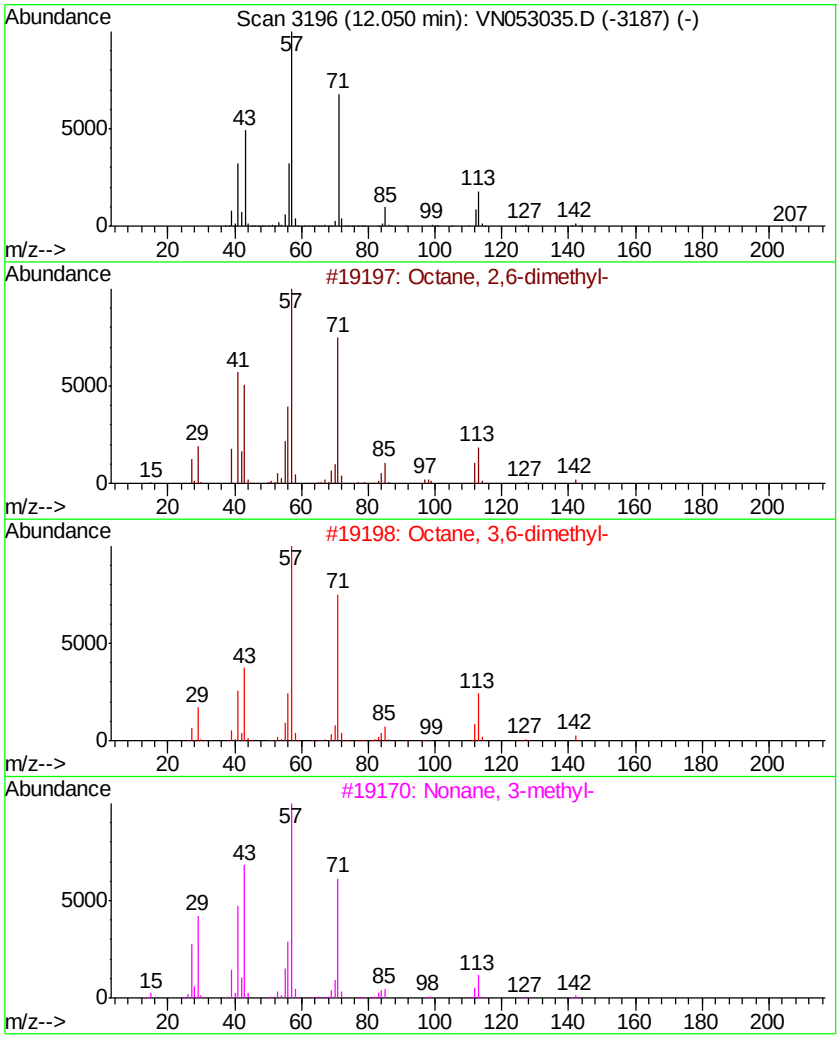
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

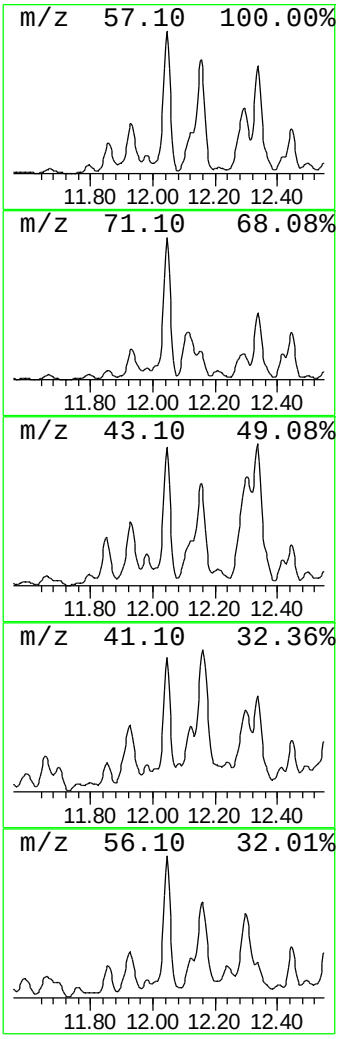
****

Peak Number 5 Octane, 2,6-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.05	131.18 ug/l	15216000	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	90
4	Sulfurous acid, 2-ethylhexyl hex...	418	C24H50O3S	1000309-19-9	64
5	Nonane, 4-methyl-5-propyl-	184	C13H28	062185-55-1	59





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Acq On : 20 Dec 2018 2:50
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ALS Vial : 42 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : EP1-SBR-4A(12-13FT)1218

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

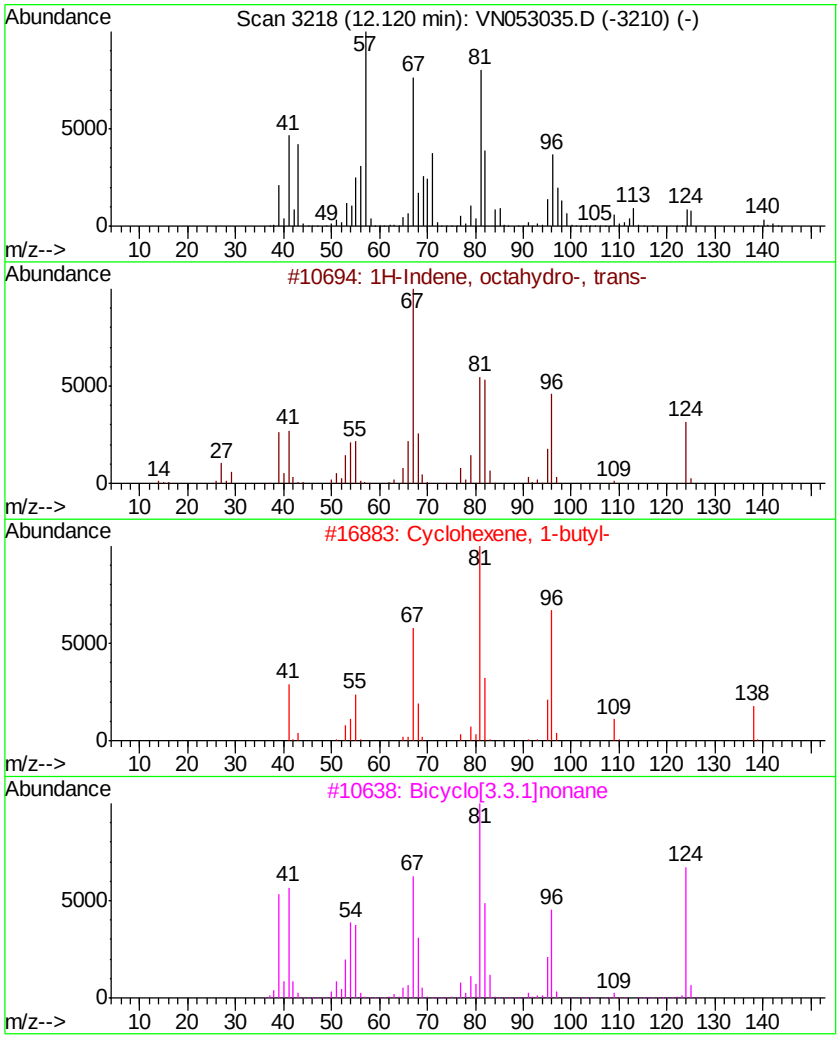
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

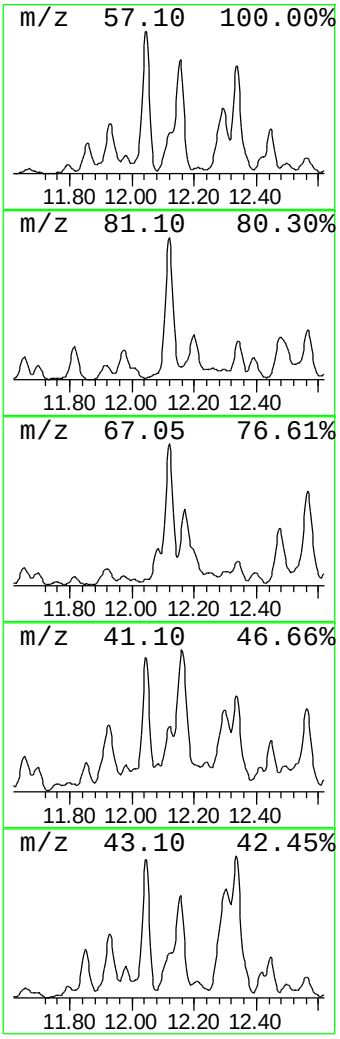
****

Peak Number 6 unknown12.12 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.12	86.07 ug/l	9983500	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, octahydro-, trans-	124	C9H16	003296-50-2	49
2	Cyclohexene, 1-butyl-	138	C10H18	003282-53-9	43
3	Bicyclo[3.3.1]nonane	124	C9H16	000280-65-9	43
4	Cyclohexene, 1-methyl-	96	C7H12	000591-49-1	38
5	3,4-Nonadiene	124	C9H16	037050-03-6	35





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN121918\
Data File : VN053035.D
Acq On : 20 Dec 2018 2:50
Operator : MD\SY
Sample : J6411-11 10X
Misc : 5.24g/5.0mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 42 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : EP1-SBR-4A(12-13FT)1218

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

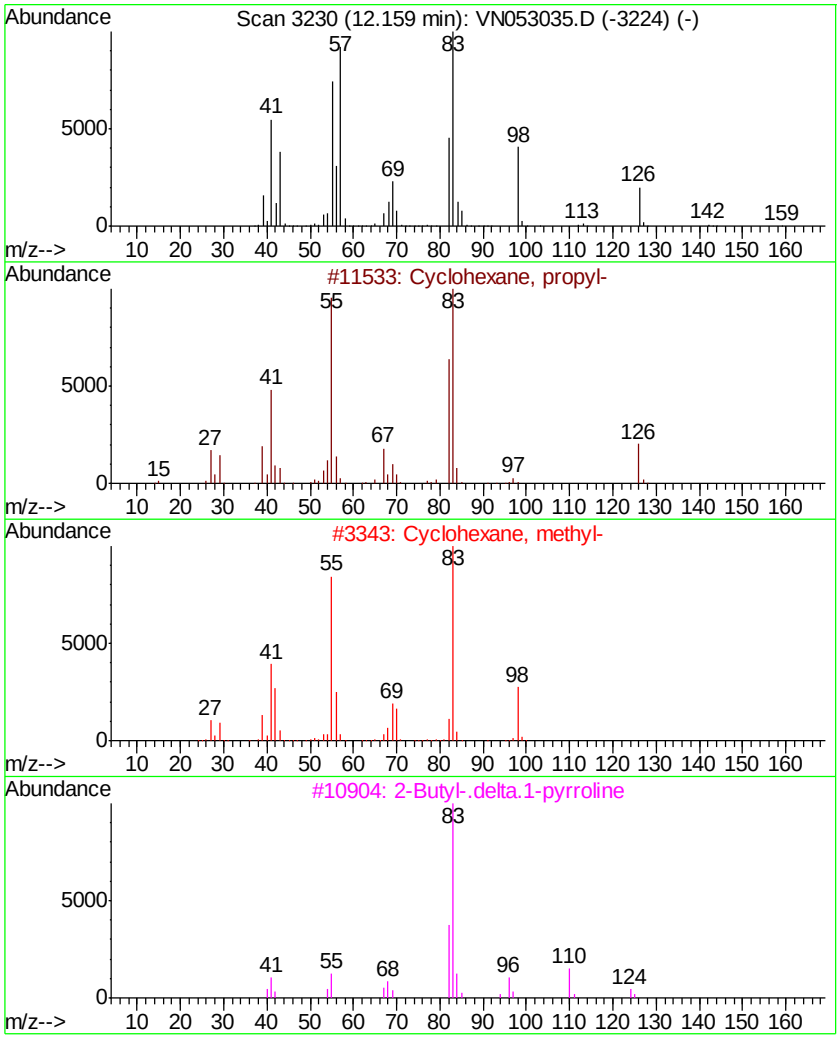
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

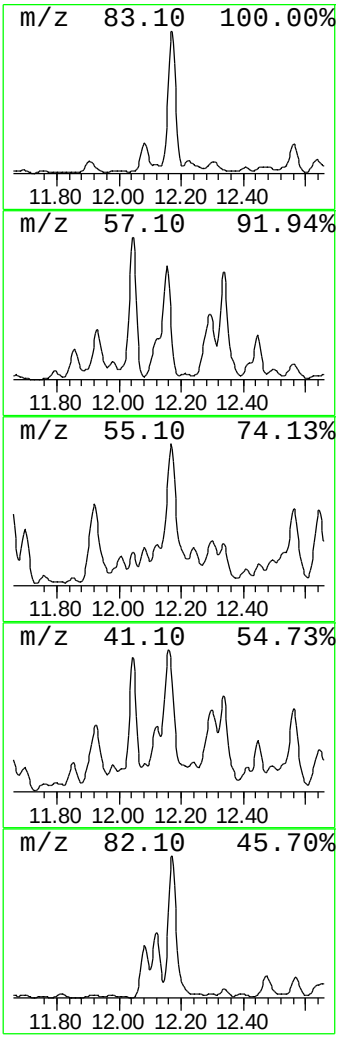
****

Peak Number 7 Cyclohexane, propyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.16	203.09 ug/l	23558100	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, propyl-	126	C9H18	001678-92-8	64
2	Cyclohexane, methyl-	98	C7H14	000108-87-2	52
3	2-Butyl-.delta.1-pyrroline	125	C8H15N	064319-86-4	50
4	1-Butene, 2,3,3-trimethyl-	98	C7H14	000594-56-9	47
5	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	43





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN121918\
Data File : VN053035.D
Acq On : 20 Dec 2018 2:50
Operator : MD\SY
Sample : J6411-11 10X
Misc : 5.24g/5.0mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 42 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : EP1-SBR-4A(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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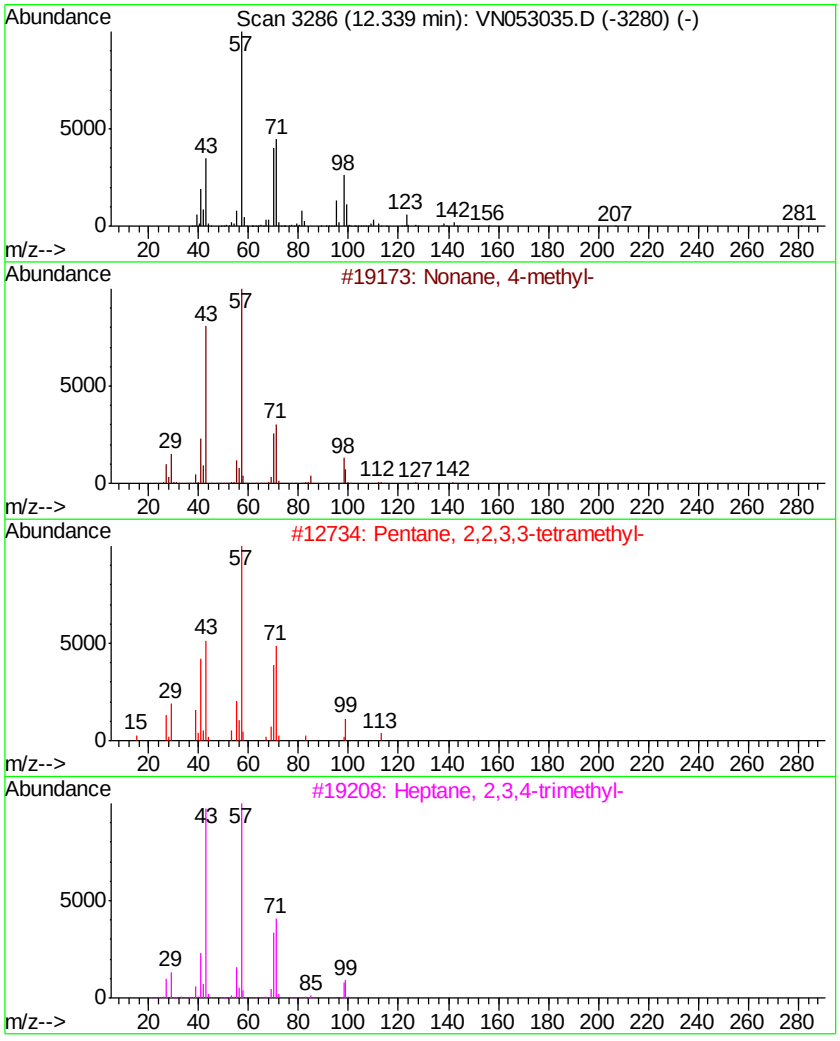
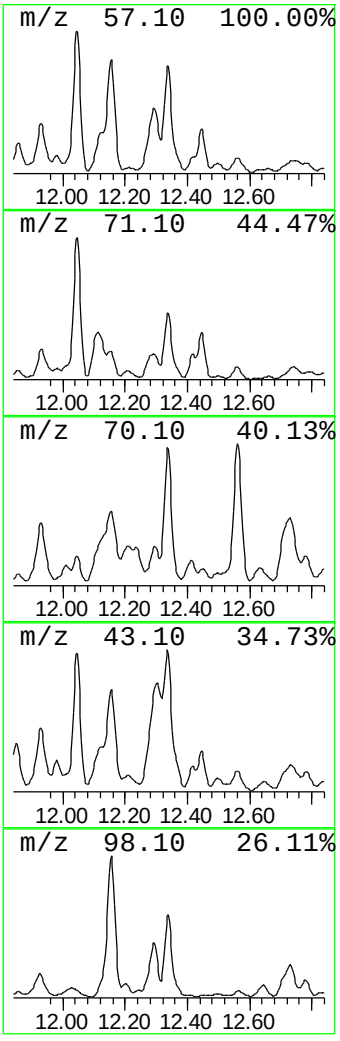
Peak Number 8 Nonane, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.34	147.05 ug/l	17057000	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonane, 4-methyl-	142	C10H22	017301-94-9	80
2	Pentane, 2,2,3,3-tetramethyl-	128	C9H20	007154-79-2	53
3	Heptane, 2,3,4-trimethyl-	142	C10H22	052896-95-4	45
4	Octane, 2,5-dimethyl-	142	C10H22	015869-89-3	36
5	Heptane, 4-propyl-	142	C10H22	003178-29-8	30





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN121918\
Data File : VN053035.D
Acq On : 20 Dec 2018 2:50
Operator : MD\SY
Sample : J6411-11 10X
Misc : 5.24g/5.0mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 42 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : EP1-SBR-4A(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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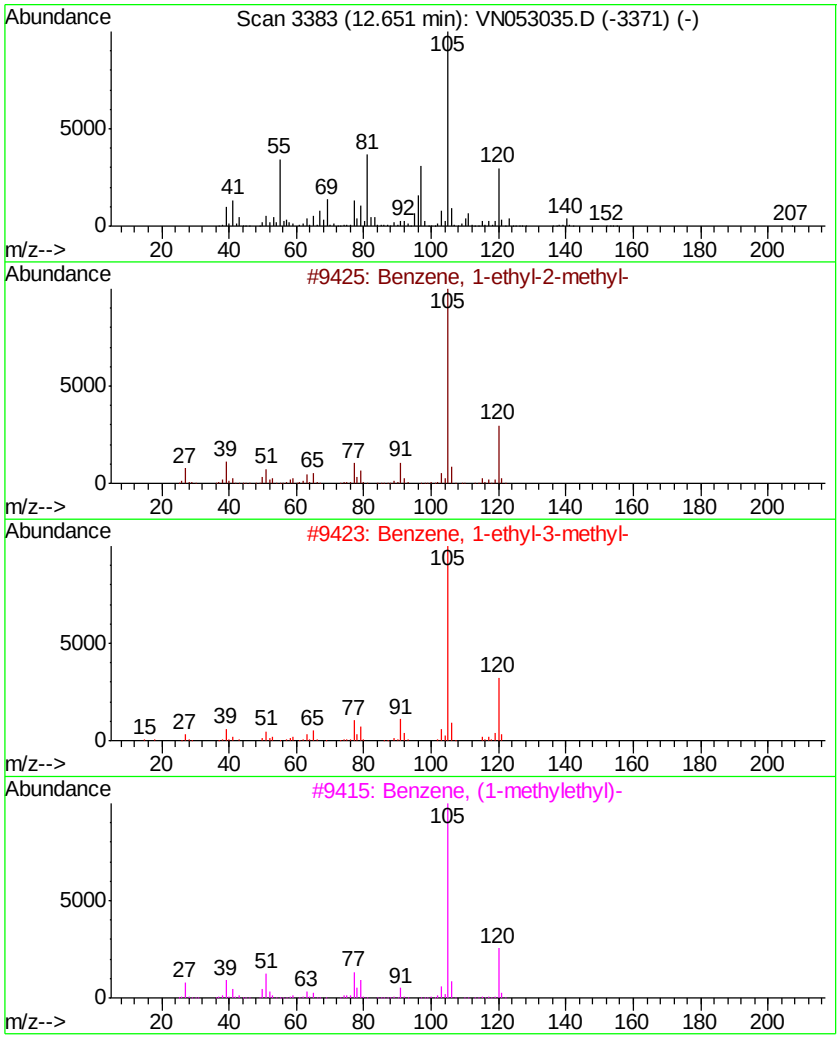
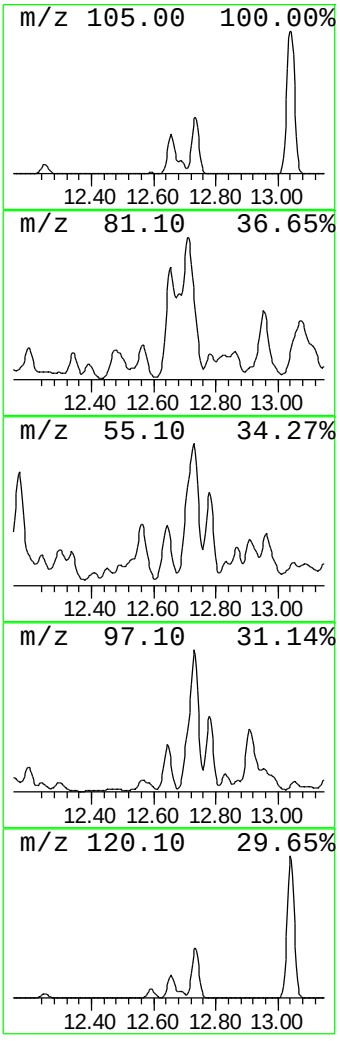
Peak Number 9 Benzene, 1-ethyl-2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.65	57.09 ug/l	20531400	1,4-Dichlorobenzene-d4	13.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	64
2	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	64
3	Benzene, (1-methylethyl)-	120	C9H12	000098-82-8	50
4	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	50
5	Mesitylene	120	C9H12	000108-67-8	45





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN121918\
Data File : VN053035.D
Acq On : 20 Dec 2018 2:50
Operator : MD\SY
Sample : J6411-11 10X
Misc : 5.24g/5.0mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 42 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : EP1-SBR-4A(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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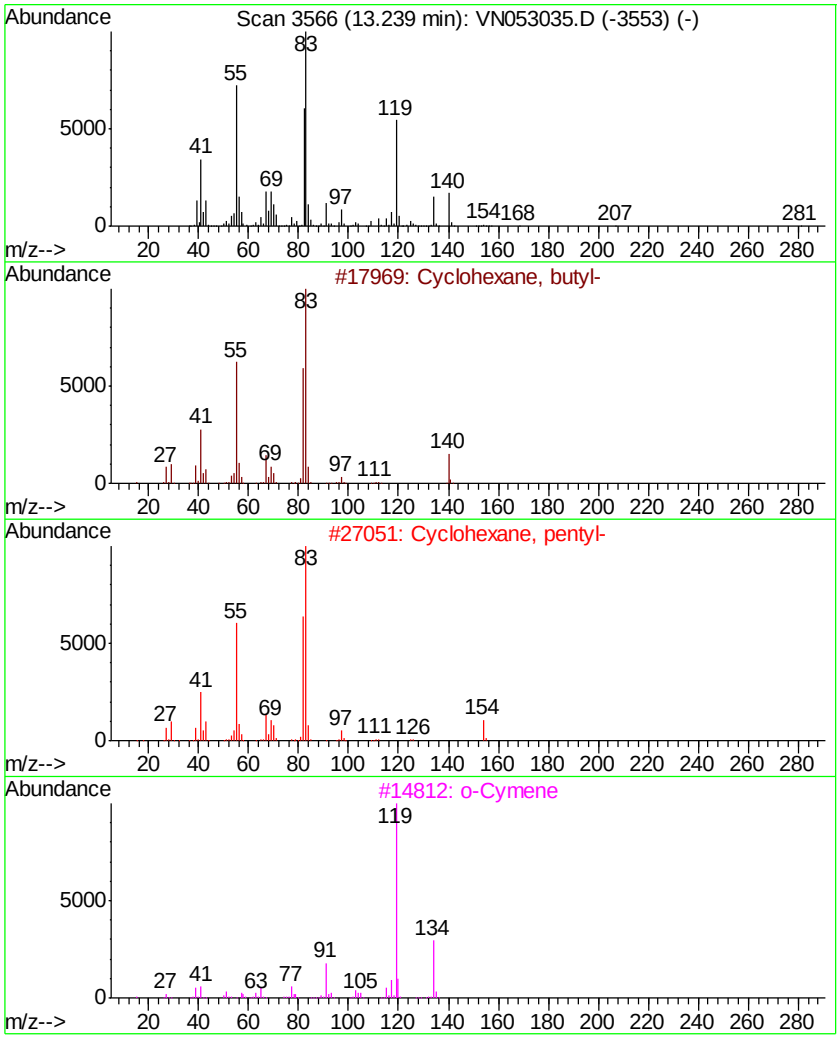
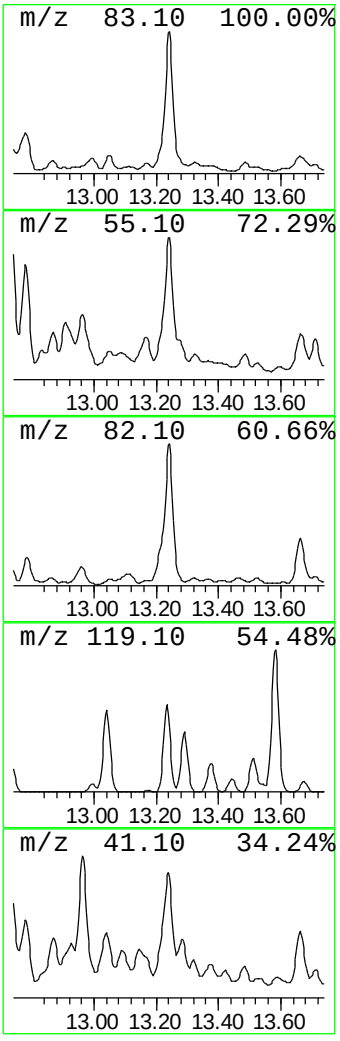
Peak Number 10 Cyclohexane, butyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.24	70.09 ug/l	25205600	1,4-Dichlorobenzene-d4	13.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, butyl-	140	C10H20	001678-93-9	92
2	Cyclohexane, pentyl-	154	C11H22	004292-92-6	64
3	o-Cymene	134	C10H14	000527-84-4	59
4	p-Cymene	134	C10H14	000099-87-6	59
5	Cyclohexane, propyl-	126	C9H18	001678-92-8	49





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN121918\
Data File : VN053035.D
Acq On : 20 Dec 2018 2:50
Operator : MD\SY
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Instrument : MSVOA_N
ClientSampleId : EP1-SBR-4A(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, 1,2,...	11.20	62.3	ug/l	7227610	3	11.41	5799810	50.0
Octane, 3-methyl-	11.30	53.2	ug/l	6173040	3	11.41	5799810	50.0
1-Ethyl-4-methylc...	11.65	72.8	ug/l	8445540	3	11.41	5799810	50.0
unknown11.92	11.92	160.2	ug/l	18579700	3	11.41	5799810	50.0
Octane, 2,6-dimet...	12.05	131.2	ug/l	15216000	3	11.41	5799810	50.0
unknown12.12	12.12	86.1	ug/l	9983500	3	11.41	5799810	50.0
Cyclohexane, propyl-	12.16	203.1	ug/l	23558100	3	11.41	5799810	50.0
Nonane, 4-methyl-	12.34	147.1	ug/l	17057000	3	11.41	5799810	50.0
Benzene, 1-ethyl-...	12.65	57.1	ug/l	20531400	4	13.35	17980700	50.0
Cyclohexane, butyl-	13.24	70.1	ug/l	25205600	4	13.35	17980700	50.0