LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA N\Data\VN121318\
Data File : VN052865.D
Acq On : 13 Dec 2018 15:34
Operator : MD\SY
Sample : J6319-03
Misc : 4.92g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 15 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : 057_BT-2-1

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\82N121218W.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	4.587	837	875	898	rBV2	124476	500690	6.04%	0.657%
2	5.047	993	1018	1052	rBV4	91370	335094	4.05%	0.440%
3	6.368	1403	1429	1446	rBV5	25914	90786	1.10%	0.119%
4	6.519	1455	1476	1492	rBV4	39462	121854	1.47%	0.160%
5	6.625	1492	1509	1525	rBV3	74561	221658	2.68%	0.291%
6	7.590	1779	1809	1817	rBV2	618559	1656820	20.00%	2.175%
7	7.661	1821	1831	1847	rVV	1447375	3687010	44.51%	4.841%
8	7.741	1847	1856	1878	rVB3	162705	426256	5.15%	0.560%
9	7.873	1878	1897	1911	rBV	442409	1082484	13.07%	1.421%
10	8.024	1928	1944	1968	rBV	679703	1595024	19.26%	2.094%
11	8.156	1968	1985	1996	rVV3	274462	703416	8.49%	0.924%
12	8.230	1998	2008	2020	rVV4	280580	775104	9.36%	1.018%
13	8.301	2020	2030	2053	rVV3	252516	719238	8.68%	0.944%
14	8.407	2055	2063	2091	rVB7	52183	149394	1.80%	0.196%
15	8.583	2100	2118	2140	rBV	2087228	4633149	55.93%	6.083%
16	8.744	2159	2168	2178	rVB2	57682	105942	1.28%	0.139%
17	8.818	2178	2191	2199	rBV2	128604	273764	3.30%	0.359%
18	9.082	2245	2273	2284	rBV3	976947	2730137	32.96%	3.585%
19	9.143	2284	2292	2307	rVB2	205218	413969	5.00%	0.544%
20	9.272	2321	2332	2344	rBV4	149323	304346	3.67%	0.400%
21	9.365	2345	2361	2375	rBV2	280406	657747	7.94%	0.864%
22	9.513	2396	2407	2419	rVB3	327250	628757	7.59%	0.826%
23	9.616	2429	2439	2445	rBV2	208463	374451	4.52%	0.492%
24	9.664	2446	2454	2462	rVB4	234549	387064	4.67%	0.508%
25	9.728	2463	2474	2480	rBV	600604	1106287	13.36%	1.453%
26	9.866	2498	2517	2540	rBV2	698052	1820026	21.97%	2.390%
27	9.973	2540	2550	2554	rBV5	99660	177005	2.14%	0.232%
28	10.021	2555	2565	2574	rVV3	358061	720065	8.69%	0.945%
29	10.088	2574	2586	2610	rVB2	4018095	8283445	100.00%	10.876%
30	10.214	2616	2625	2630	rBV3	191783	318381	3.84%	0.418%
31	10.259	2631	2639	2642	rBV2	294671	436175	5.27%	0.573%
32	10.345	2659	2666	2671	rBV4	62594	97164	1.17%	0.128%
33	10.387	2672	2679	2685	rVV3	183755	288850	3.49%	0.379%
34	10.432	2685	2693	2709	rVB	524478	915590	11.05%	1.202%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA N\Data\VN121318\
Data File : VN052865.D
Acq On : 13 Dec 2018 15:34
Operator : MD\SY
Sample : J6319-03
Misc : 4.92g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 15 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : 057_BT-2-1

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\82N121218W.M
Title : SW846 8260

35	10.522	2709	2721	2735	rBV5	764012	1754649	21.18%	2.304%
36	10.625	2745	2753	2762	rVB5	259407	461004	5.57%	0.605%
37	10.718	2763	2782	2792	rBV	554177	1078449	13.02%	1.416%
38	10.821	2792	2814	2825	rVV2	506462	1394652	16.84%	1.831%
39	10.882	2826	2833	2838	rVV4	273230	484740	5.85%	0.636%
40	10.918	2839	2844	2848	rVV3	368543	562615	6.79%	0.739%
41	10.950	2849	2854	2862	rVV	647730	1111522	13.42%	1.459%
42	11.005	2863	2871	2881	rVV2	748065	1449416	17.50%	1.903%
43	11.062	2882	2889	2897	rVV5	291873	543878	6.57%	0.714%
44	11.120	2898	2907	2915	rVV4	421803	786506	9.49%	1.033%
45	11.201	2916	2932	2952	rVB6	1136437	3100511	37.43%	4.071%
46	11.300	2952	2963	2984	rBV	899614	1901603	22.96%	2.497%
47	11.407	2985	2996	3015	rBV	2713600	4784494	57.76%	6.282%
48	11.593	3045	3054	3063	rBV6	270579	547131	6.61%	0.718%
49	11.654	3065	3073	3081	rVV	445825	736263	8.89%	0.967%
50	11.751	3096	3103	3111	rBV8	119927	216577	2.61%	0.284%
51	11.812	3114	3122	3128	rBV5	114295	189251	2.28%	0.248%
52	11.857	3129	3136	3144	rVB6	164129	247834	2.99%	0.325%
53	11.924	3145	3157	3168	rBV5	541569	1287982	15.55%	1.691%
54	12.043	3188	3194	3202	rVB	465990	611276	7.38%	0.803%
55	12.117	3210	3217	3223	rBV3	385059	607526	7.33%	0.798%
56	12.162	3225	3231	3240	rVB5	477392	789333	9.53%	1.036%
57	12.400	3297	3305	3314	rVV	2044633	3217478	38.84%	4.224%
58	12.445	3315	3319	3326	rVB2	305294	350796	4.23%	0.461%
59	12.561	3350	3355	3359	rBV5	156810	204989	2.47%	0.269%
60	12.728	3397	3407	3416	rBV7	266642	542738	6.55%	0.713%
61	12.924	3461	3468	3473	rBV5	272321	390733	4.72%	0.513%
62	12.963	3474	3480	3494	rVB3	481332	805642	9.73%	1.058%
63	13.091	3513	3520	3530	rBV	269007	433624	5.23%	0.569%
64	13.345	3587	3599	3610	rVB	2640390	4498168	54.30%	5.906%
65	13.513	3646	3651	3656	rBV	194367	274582	3.31%	0.361%
66	13.889	3760	3768	3777	rBV	697868	1041620	12.57%	1.368%
67	13.995	3793	3801	3810	rVB2	657986	1031698	12.45%	1.355%
68	14.297	3888	3895	3901	rBV3	274072	411965	4.97%	0.541%
69	14.593	3978	3987	3996	rBV4	508761	991001	11.96%	1.301%
70	14.644	3998	4003	4014	rVB3	358007	584232	7.05%	0.767%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA N\Data\VN121318\
Data File : VN052865.D
Acq On : 13 Dec 2018 15:34
Operator : MD\SY
Sample : J6319-03
Misc : 4.92g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 15 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : 057_BT-2-1

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\82N121218W.M
Title : SW846 8260

Sum of corrected areas: 76163620

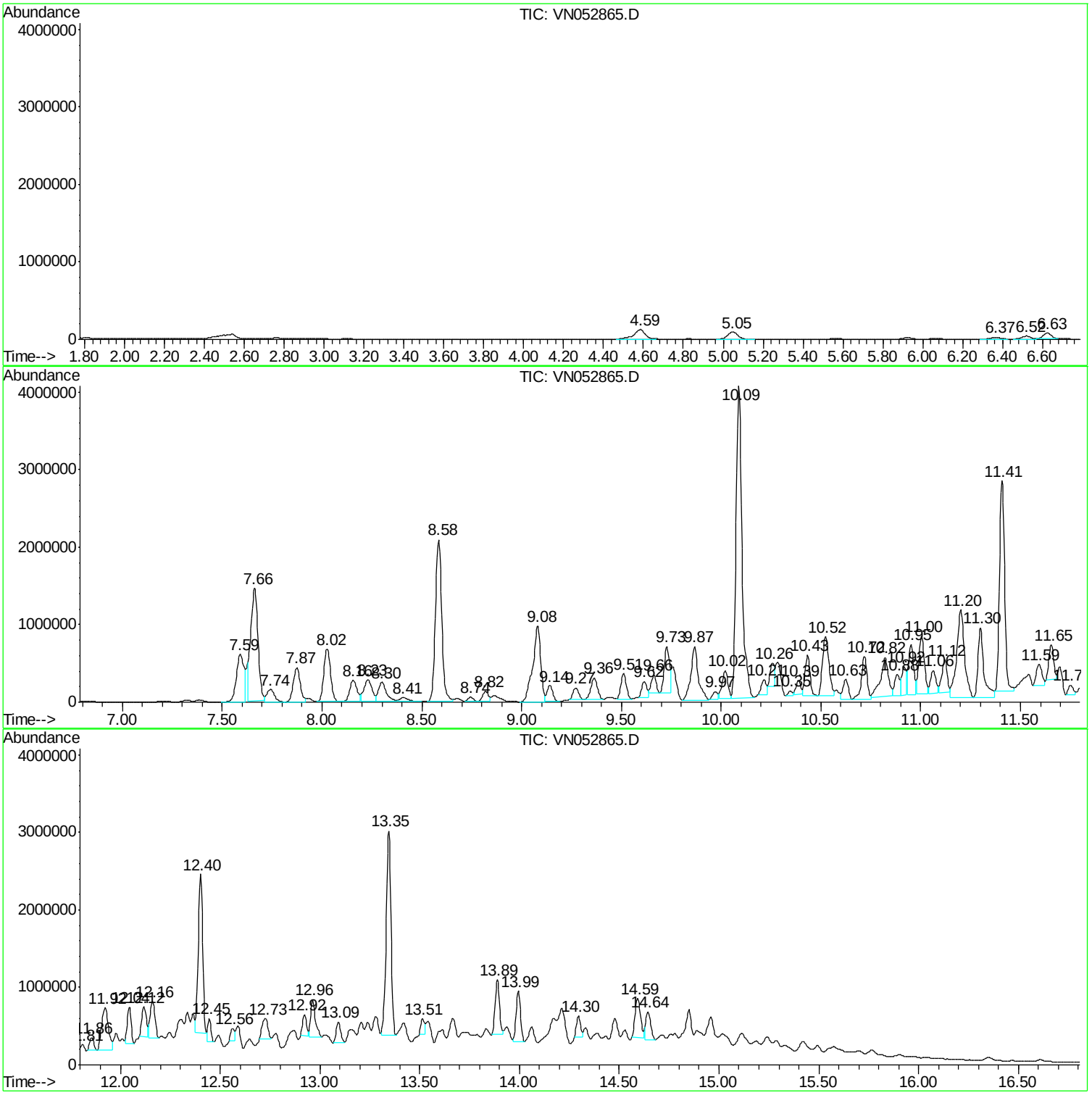
LSC Report - Integrated Chromatogram

Data Path : Z:\voasrv\HPCHEM1\MSVOA N\Data\VN121318\
Data File : VN052865.D
Acq On : 13 Dec 2018 15:34
Operator : MD\SY
Sample : J6319-03
Misc : 4.92g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 15 Sample Multiplier: 28

Instrument :
MSVOA_N
ClientSampleId :
057_BT-2-1

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N121218W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121318\
Data File : VN052865.D
Acq On : 13 Dec 2018 15:34
Operator : MD\SY
Sample : J6319-03
Misc : 4.92g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 15 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : 057_BT-2-1

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N121218W.M
Quant Title : SW846 8260

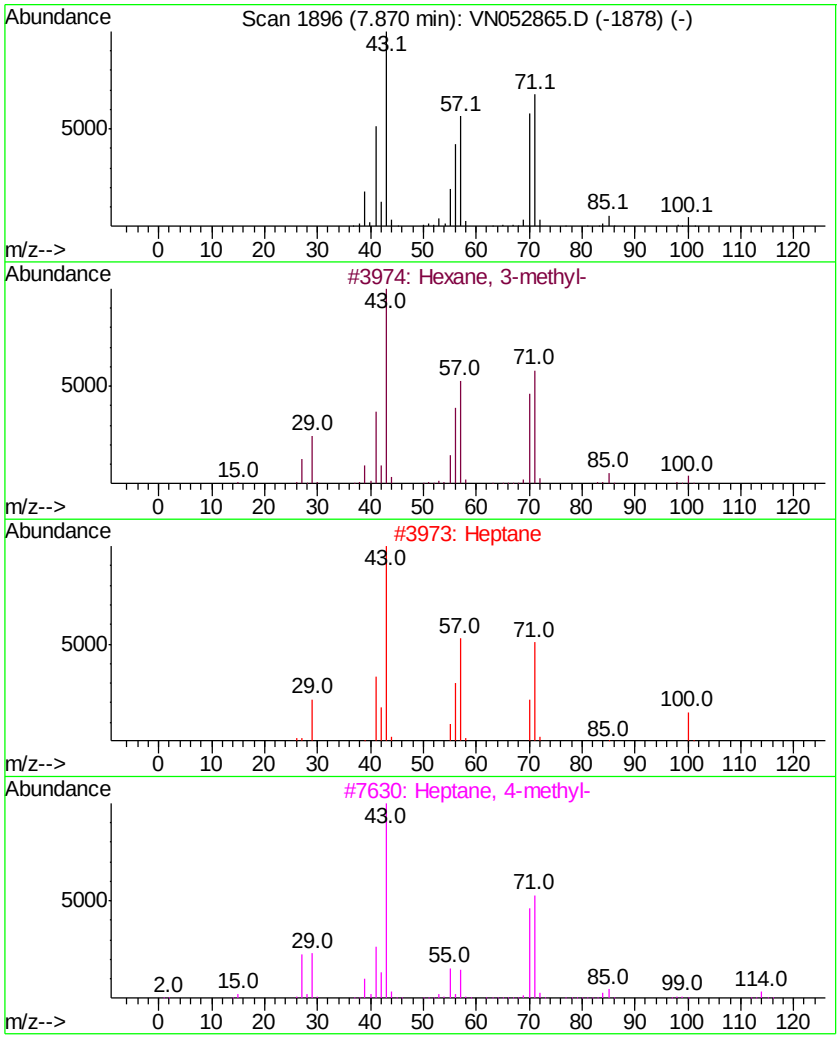
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

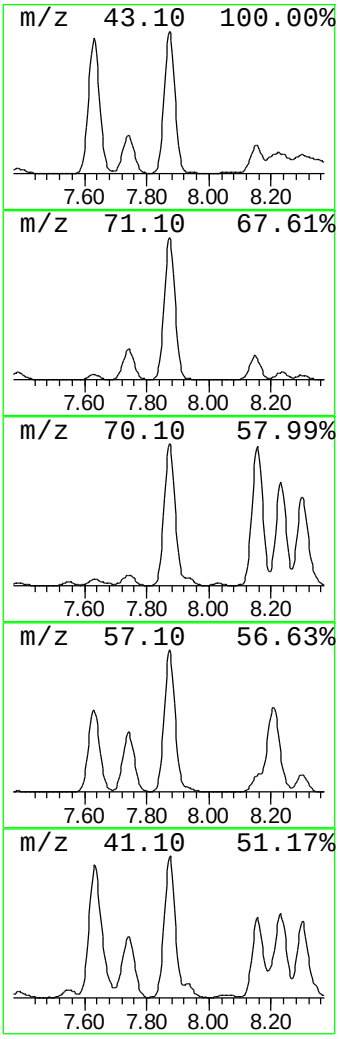
****

Peak Number 1 Hexane, 3-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.87	14.68 ug/l	1082480	Pentafluorobenzene	7.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 3-methyl-	100	C7H16	000589-34-4	94
2	Heptane	100	C7H16	000142-82-5	80
3	Heptane, 4-methyl-	114	C8H18	000589-53-7	59
4	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	53
5	Heptane, 3,3,4-trimethyl-	142	C10H22	020278-87-9	53





Library Search Compound Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA N\Data\VN121318\
Data File : VN052865.D
Acq On : 13 Dec 2018 15:34
Operator : MD\SY
Sample : J6319-03
Misc : 4.92g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 15 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : 057_BT-2-1

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N121218W.M
Quant Title : SW846 8260

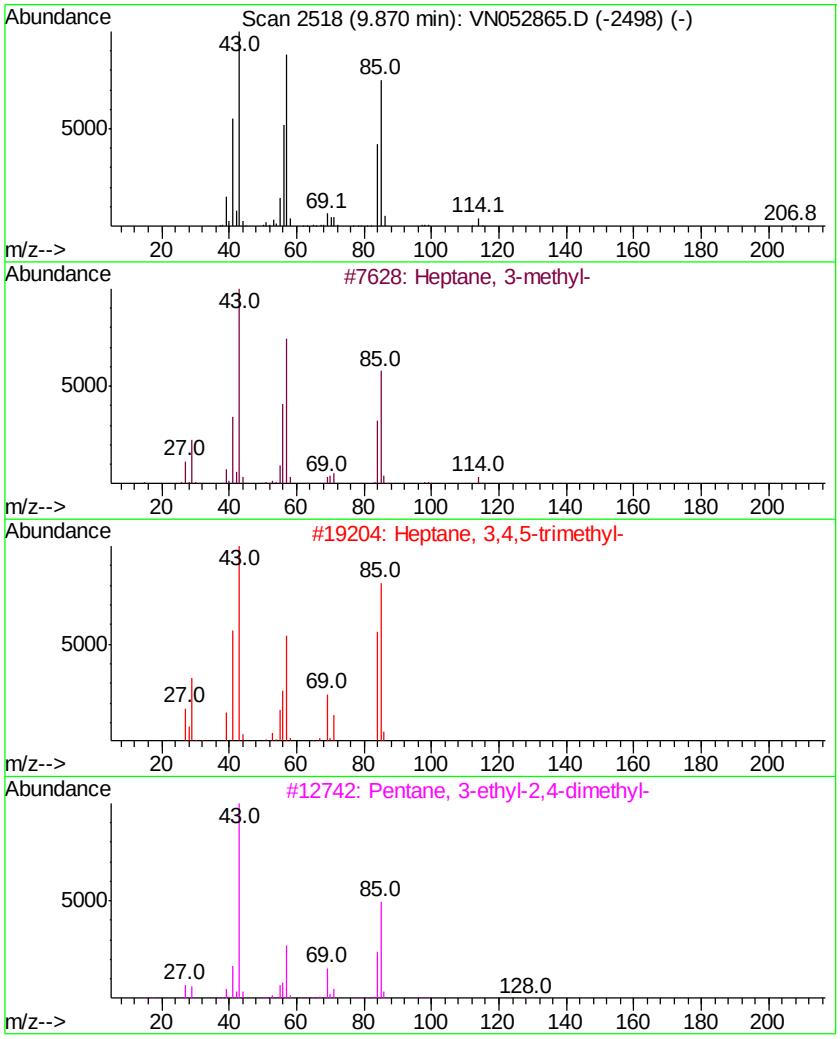
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

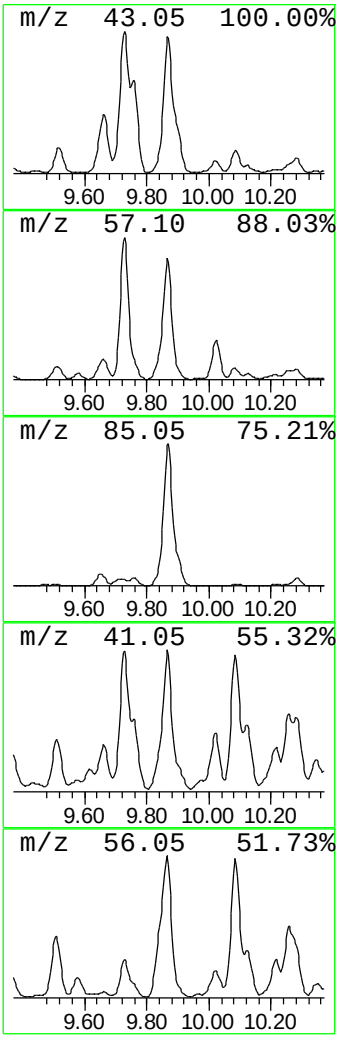
****

Peak Number 3 Heptane, 3-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.87	19.64 ug/l	1820030	1,4-Difluorobenzene	8.58

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane, 3-methyl-	114	C8H18	000589-81-1	87
2	Heptane, 3,4,5-trimethyl-	142	C10H22	020278-89-1	72
3	Pentane, 3-ethyl-2,4-dimethyl-	128	C9H20	001068-87-7	64
4	Hexane, 1-(hexyloxy)-2-methyl-	200	C13H28O	074421-17-3	64
5	Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	53





Data Path : Z:\voasrv\HPCHEM1\MSVOA N\Data\VN121318\
Data File : VN052865.D
Acq On : 13 Dec 2018 15:34
Operator : MD\SY
Sample : J6319-03
Misc : 4.92g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 15 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : 057_BT-2-1

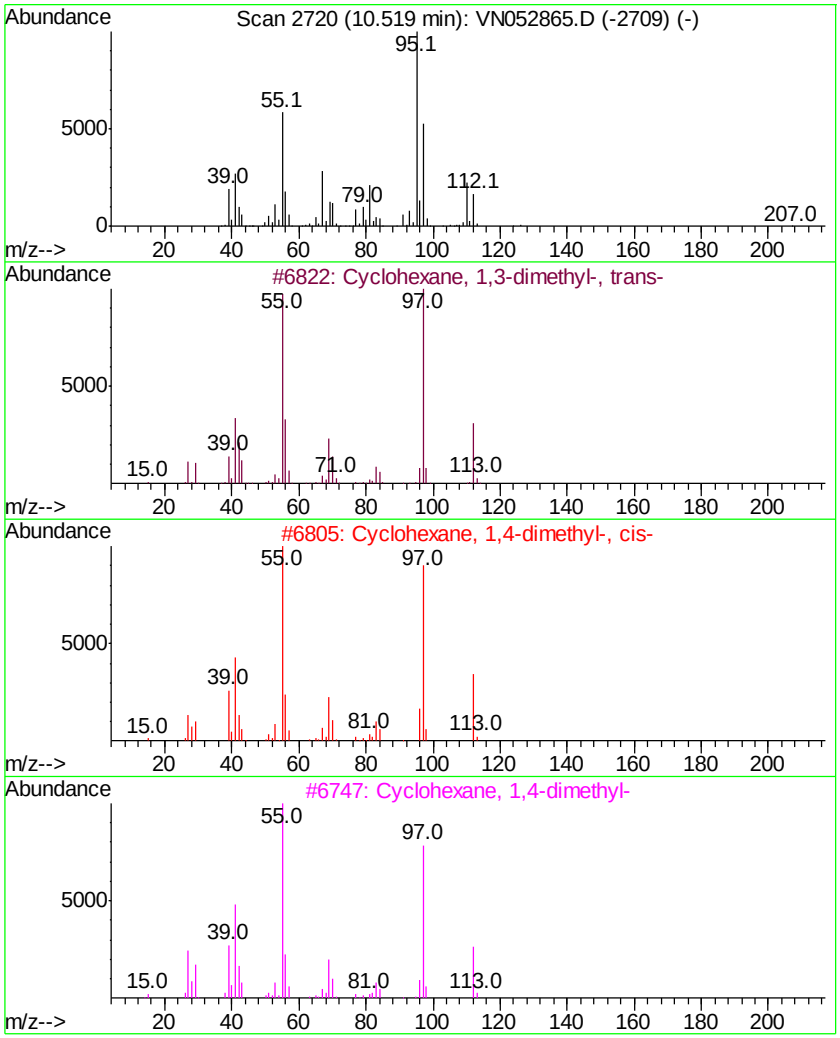
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N121218W.M
Quant Title : SW846 8260

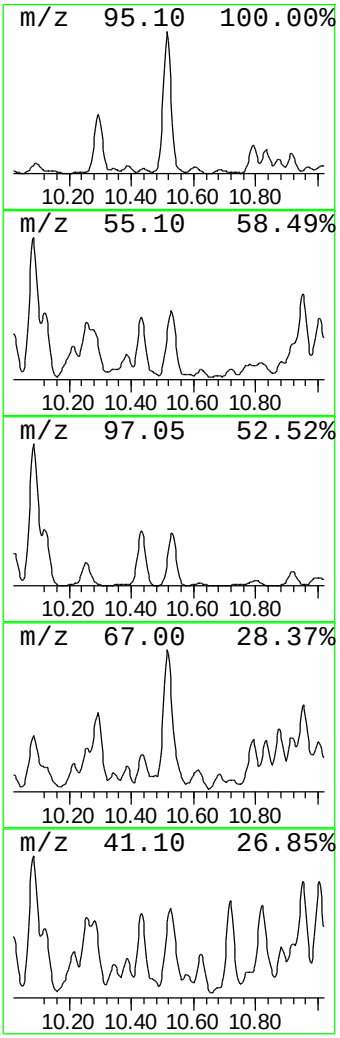
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.52	18.34 ug/l	1754650	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,3-dimethyl-, trans-	112	C8H16	002207-03-6	87
2	Cyclohexane, 1,4-dimethyl-, cis-	112	C8H16	000624-29-3	55
3	Cyclohexane, 1,4-dimethyl-	112	C8H16	000589-90-2	55
4	Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	50
5	Cyclohexane, 1,4-dimethyl-, trans-	112	C8H16	002207-04-7	45





Library Search Compound Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121318\
Data File : VN052865.D
Acq On : 13 Dec 2018 15:34
Operator : MD\SY
Sample : J6319-03
Misc : 4.92g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 15 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : 057_BT-2-1

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N121218W.M
Quant Title : SW846 8260

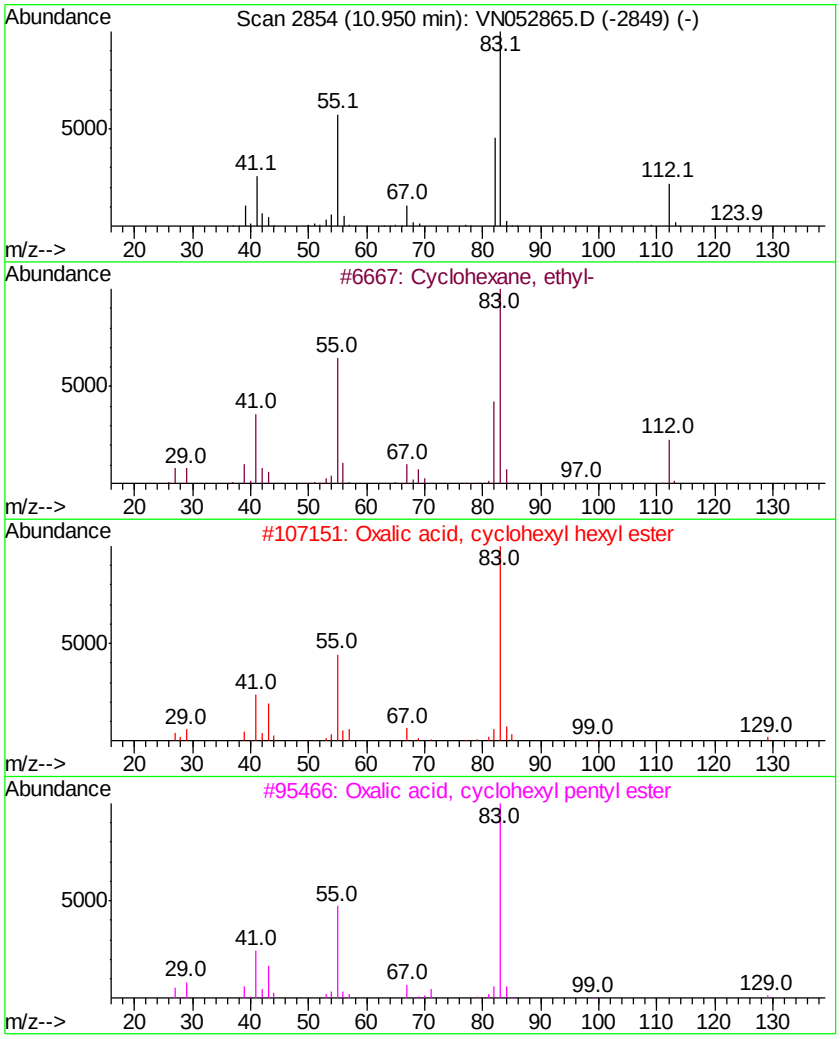
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

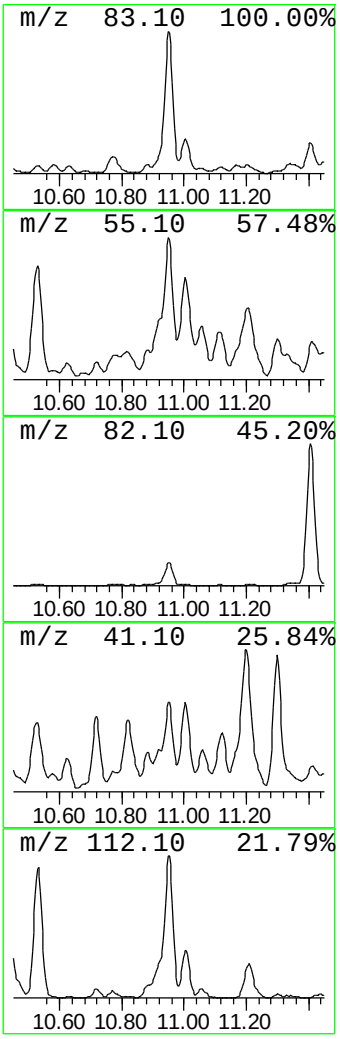
****

Peak Number 6 Cyclohexane, ethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.95	11.62 ug/l	1111520	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, ethyl-	112	C8H16	001678-91-7	91
2	Oxalic acid, cyclohexyl hexyl ester	256	C14H24O4	1000309-30-8	50
3	Oxalic acid, cyclohexyl pentyl e...	242	C13H22O4	1000309-30-6	50
4	Oxalic acid, cyclohexyl butyl ester	228	C12H20O4	1000309-30-5	50
5	Oxalic acid, cyclohexyl propyl e...	214	C11H18O4	1000309-30-3	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121318\
Data File : VN052865.D
Acq On : 13 Dec 2018 15:34
Operator : MD\SY
Sample : J6319-03
Misc : 4.92g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 15 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : 057_BT-2-1

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N121218W.M
Quant Title : SW846 8260

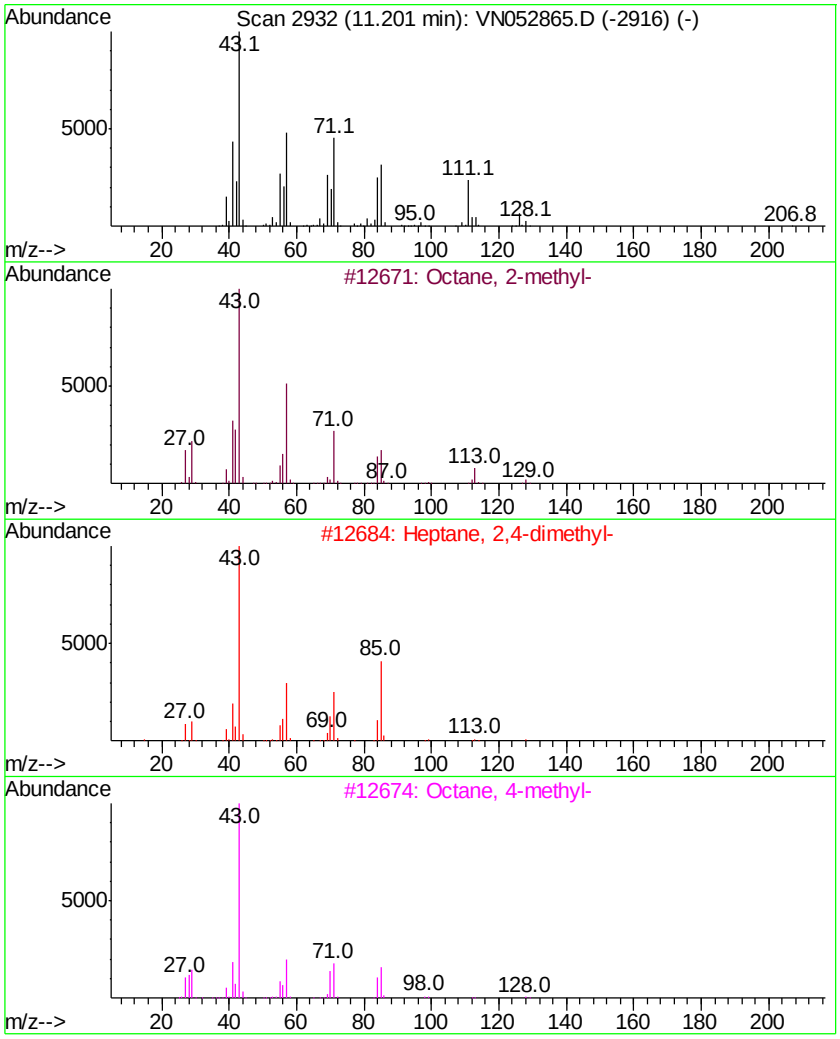
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

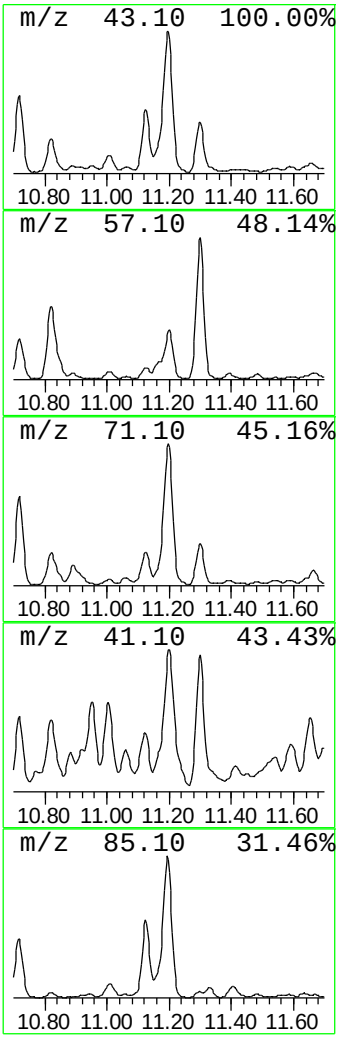
****

Peak Number 8 Octane, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.20	32.40 ug/l	3100510	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2-methyl-	128	C9H20	003221-61-2	58
2	Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	47
3	Octane, 4-methyl-	128	C9H20	002216-34-4	43
4	Octane	114	C8H18	000111-65-9	43
5	Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121318\
Data File : VN052865.D
Acq On : 13 Dec 2018 15:34
Operator : MD\SY
Sample : J6319-03
Misc : 4.92g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 15 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : 057_BT-2-1

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N121218W.M
Quant Title : SW846 8260

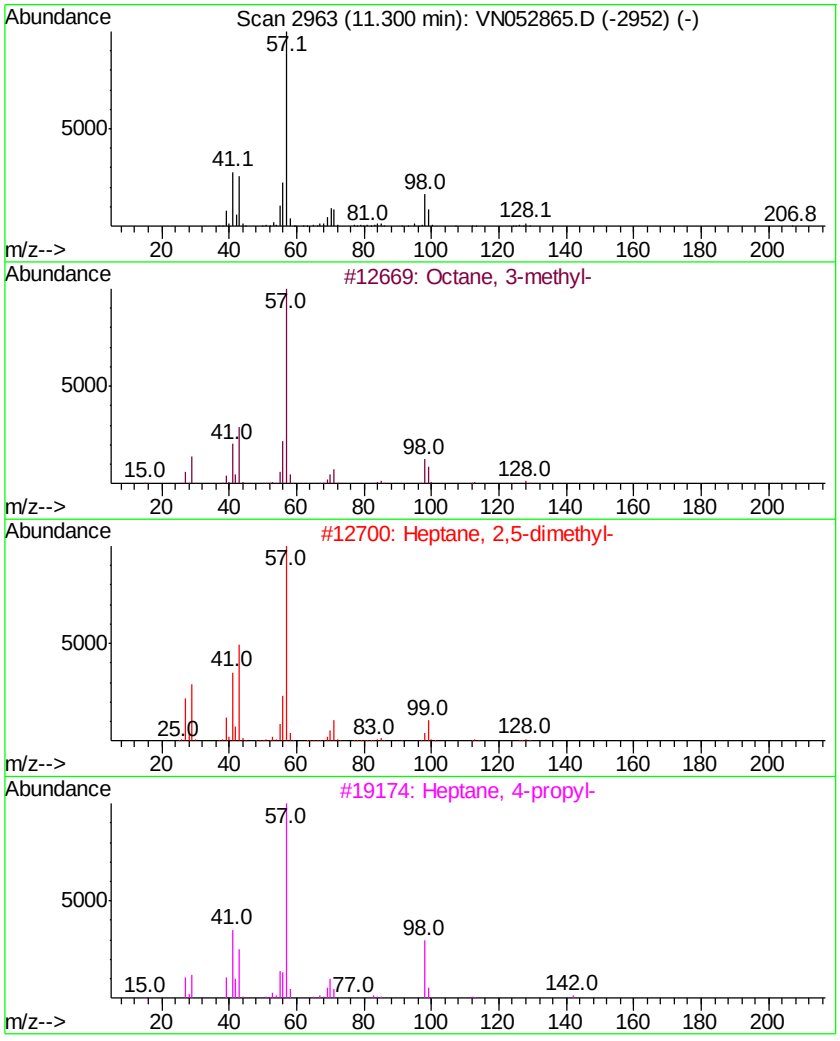
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

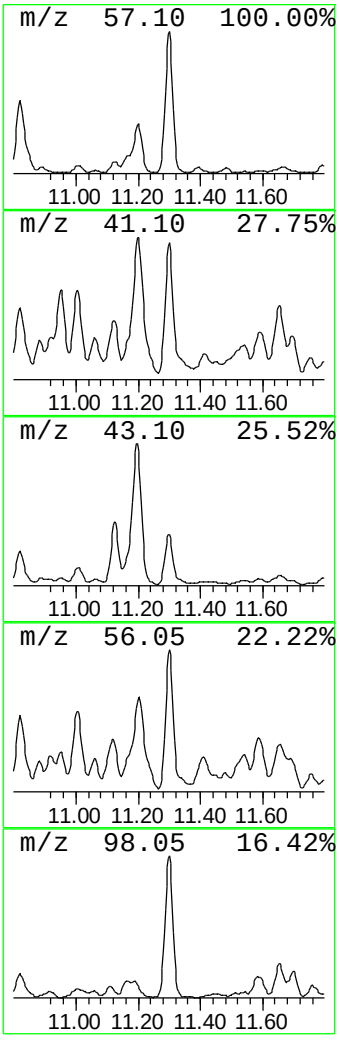
****

Peak Number 9 Octane, 3-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.30	19.87 ug/l	1901600	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 3-methyl-	128	C9H20	002216-33-3	87
2	Heptane, 2,5-dimethyl-	128	C9H20	002216-30-0	72
3	Heptane, 4-propyl-	142	C10H22	003178-29-8	59
4	Heptane, 3,5-dimethyl-	128	C9H20	000926-82-9	58
5	Heptane, 3-ethyl-	128	C9H20	015869-80-4	52





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121318\
Data File : VN052865.D
Acq On : 13 Dec 2018 15:34
Operator : MD\SY
Sample : J6319-03
Misc : 4.92g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 15 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : 057_BT-2-1

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N121218W.M
Quant Title : SW846 8260

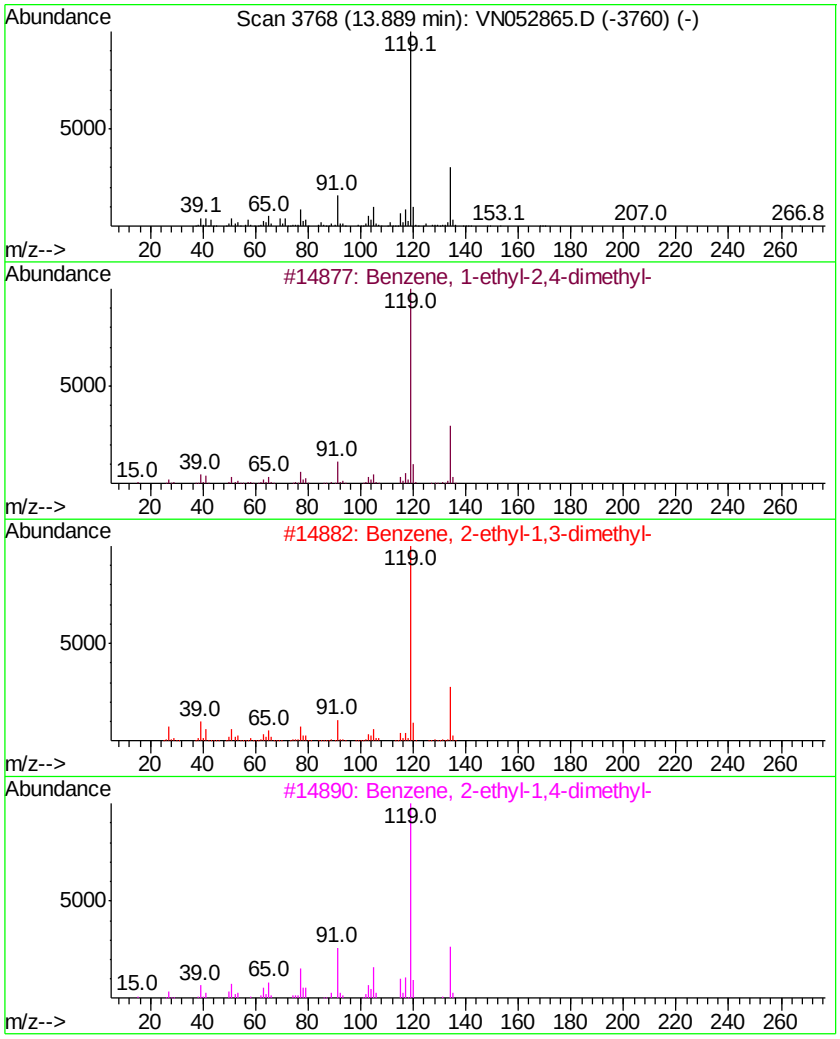
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

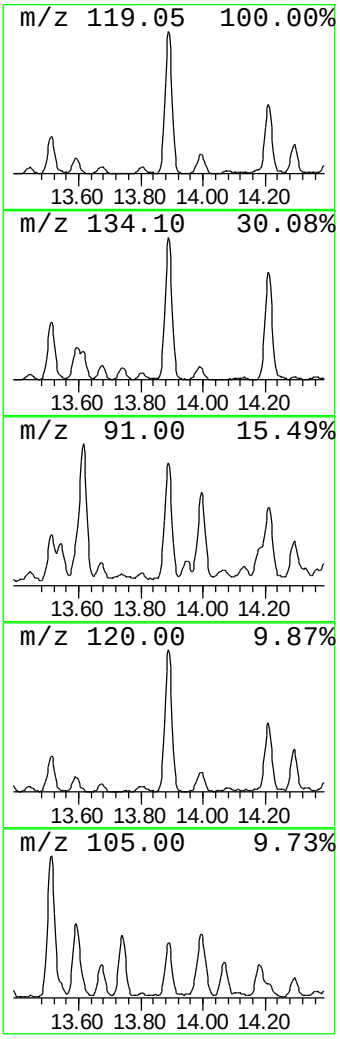
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	11.58 ug/l	1041620	1,4-Dichlorobenzene-d4	13.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	97
2	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	95
3	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	95
4	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	94
5	o-Cymene	134	C10H14	000527-84-4	94





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121318\
Data File : VN052865.D
Acq On : 13 Dec 2018 15:34
Operator : MD\SY
Sample : J6319-03
Misc : 4.92g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 15 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : 057_BT-2-1

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N121218W.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
Hexane, 3-methyl-	7.87	14.7	ug/l	1082480	1	7.66	3687010	50.0
Heptane, 3-methyl-	9.87	19.6	ug/l	1820030	2	8.58	4633150	50.0
Cyclohexane, 1,3-...	10.52	18.3	ug/l	1754650	3	11.41	4784490	50.0
Cyclohexane, ethyl-	10.95	11.6	ug/l	1111520	3	11.41	4784490	50.0
Octane, 2-methyl-	11.20	32.4	ug/l	3100510	3	11.41	4784490	50.0
Octane, 3-methyl-	11.30	19.9	ug/l	1901600	3	11.41	4784490	50.0
Benzene, 1-ethyl-...	13.89	11.6	ug/l	1041620	4	13.35	4498170	50.0