LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN020320\
Data File : VN059980.D
Acq On : 3 Feb 2020 17:19
Operator : JC/MD
Sample : L1346-05 20X
Misc : 6.46g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : PD-3-(35-37)

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\82N011320W.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	2.420	190	201	233	rVB7	13696	42902	3.76%	0.492%
2	4.564	862	868	890	rVB3	14091	39994	3.51%	0.458%
3	5.027	992	1012	1036	rVB3	12682	43425	3.81%	0.498%
4	5.548	1155	1174	1190	rBV4	10875	31937	2.80%	0.366%
5	6.497	1452	1469	1486	rBV6	7511	24183	2.12%	0.277%
6	6.606	1486	1503	1519	rVB6	7006	21489	1.88%	0.246%
7	7.567	1782	1802	1812	rBV	133311	348022	30.52%	3.989%
8	7.644	1814	1826	1841	rVV	262361	673709	59.08%	7.721%
9	7.722	1842	1850	1868	rVB3	25818	64729	5.68%	0.742%
10	7.857	1876	1892	1908	rBV3	50443	124128	10.89%	1.423%
11	8.008	1921	1939	1956	rBV	139837	330694	29.00%	3.790%
12	8.140	1965	1980	1990	rBV5	20579	51423	4.51%	0.589%
13	8.214	1992	2003	2015	rVV7	19657	56533	4.96%	0.648%
14	8.284	2015	2025	2045	rVB4	13062	34005	2.98%	0.390%
15	8.419	2048	2067	2083	rVB2	33398	71721	6.29%	0.822%
16	8.567	2097	2113	2136	rBV	373772	796277	69.83%	9.126%
17	8.805	2177	2187	2196	rBV4	8105	17049	1.50%	0.195%
18	9.066	2245	2268	2280	rBV3	64713	169529	14.87%	1.943%
19	9.130	2280	2288	2300	rVB3	16174	32442	2.85%	0.372%
20	9.255	2317	2327	2337	rVB4	12236	23477	2.06%	0.269%
21	9.352	2340	2357	2373	rBV6	12788	33669	2.95%	0.386%
22	9.500	2392	2403	2414	rBV4	19141	39908	3.50%	0.457%
23	9.603	2427	2435	2440	rBV4	10728	17795	1.56%	0.204%
24	9.651	2443	2450	2460	rVB6	16046	27983	2.45%	0.321%
25	9.718	2460	2471	2478	rBV	42305	83095	7.29%	0.952%
26	9.857	2495	2514	2537	rBV	50194	127191	11.15%	1.458%
27	10.008	2552	2561	2569	rVV5	9713	20625	1.81%	0.236%
28	10.078	2569	2583	2605	rVB	608610	1140292	100.00%	13.069%
29	10.201	2606	2621	2628	rBV5	12159	27510	2.41%	0.315%
30	10.275	2629	2644	2656	rVV6	45330	106333	9.33%	1.219%
31	10.422	2683	2690	2698	rVB4	13813	22116	1.94%	0.253%
32	10.513	2707	2718	2733	rBV6	33641	74415	6.53%	0.853%
33	10.615	2742	2750	2760	rVB6	11744	22506	1.97%	0.258%
34	10.712	2760	2780	2789	rBV3	17935	37280	3.27%	0.427%

LSC Area Percent Report

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Misc : 6.46g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : PD-3-(35-37)

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

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Peak separation: 5

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Title : SW846 8260

35	10.779	2789	2801	2803	rVV7	6956	14187	1.24%	0.163%
36	10.815	2804	2812	2823	rVV2	19940	43008	3.77%	0.493%
37	10.873	2823	2830	2835	rVV10	10573	18876	1.66%	0.216%
38	10.908	2837	2841	2846	rVV3	15370	22815	2.00%	0.261%
39	10.943	2847	2852	2860	rVV2	19727	34676	3.04%	0.397%
40	10.998	2861	2869	2878	rVV5	19559	39054	3.42%	0.448%
41	11.056	2881	2887	2896	rVV9	10077	19652	1.72%	0.225%
42	11.117	2897	2906	2913	rVV5	12342	22344	1.96%	0.256%
43	11.194	2914	2930	2950	rVB5	45769	118757	10.41%	1.361%
44	11.297	2950	2962	2972	rBV	37368	69875	6.13%	0.801%
45	11.400	2981	2994	3010	rBV	547815	948777	83.20%	10.874%
46	11.586	3044	3052	3060	rBV10	7496	13831	1.21%	0.159%
47	11.651	3062	3072	3081	rVV6	13138	26068	2.29%	0.299%
48	11.924	3144	3157	3168	rBV5	12307	30221	2.65%	0.346%
49	12.043	3187	3194	3201	rVB3	9907	12682	1.11%	0.145%
50	12.114	3208	3216	3222	rBV9	8401	13243	1.16%	0.152%
51	12.397	3293	3304	3316	rVB	429790	703922	61.73%	8.067%
52	12.586	3356	3363	3373	rVB	40747	63739	5.59%	0.730%
53	12.721	3386	3405	3416	rBV	10525	28503	2.50%	0.327%
54	12.959	3474	3479	3491	rVB6	9976	16136	1.42%	0.185%
55	13.152	3529	3539	3550	rBV7	9875	25985	2.28%	0.298%
56	13.284	3573	3580	3585	rBV5	9405	12013	1.05%	0.138%
57	13.339	3585	3597	3617	rVV	556239	959264	84.12%	10.994%
58	13.509	3642	3650	3657	rBV2	28481	45293	3.97%	0.519%
59	13.590	3668	3675	3680	rBV2	17937	29981	2.63%	0.344%
60	13.670	3692	3700	3708	rBV7	10526	17765	1.56%	0.204%
61	13.741	3714	3722	3732	rVB	19442	30318	2.66%	0.347%
62	13.885	3758	3767	3777	rBV	90654	139597	12.24%	1.600%
63	13.940	3779	3784	3791	rVV7	14185	20985	1.84%	0.241%
64	13.991	3792	3800	3812	rVB	47739	73964	6.49%	0.848%
65	14.127	3836	3842	3848	rBV3	12283	20420	1.79%	0.234%
66	14.207	3860	3867	3878	rVB	41971	64206	5.63%	0.736%
67	14.294	3888	3894	3901	rBV4	22628	33679	2.95%	0.386%
68	14.474	3943	3950	3960	rBV2	35009	61230	5.37%	0.702%
69	14.590	3976	3986	3996	rBV3	62607	131889	11.57%	1.512%
70	14.644	3999	4003	4007	rBV2	17357	20158	1.77%	0.231%

LSC Area Percent Report

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ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : PD-3-(35-37)

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\82N011320W.M
Title : SW846 8260

Sum of corrected areas: 8725499

LSC Report - Integrated Chromatogram

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN020320\
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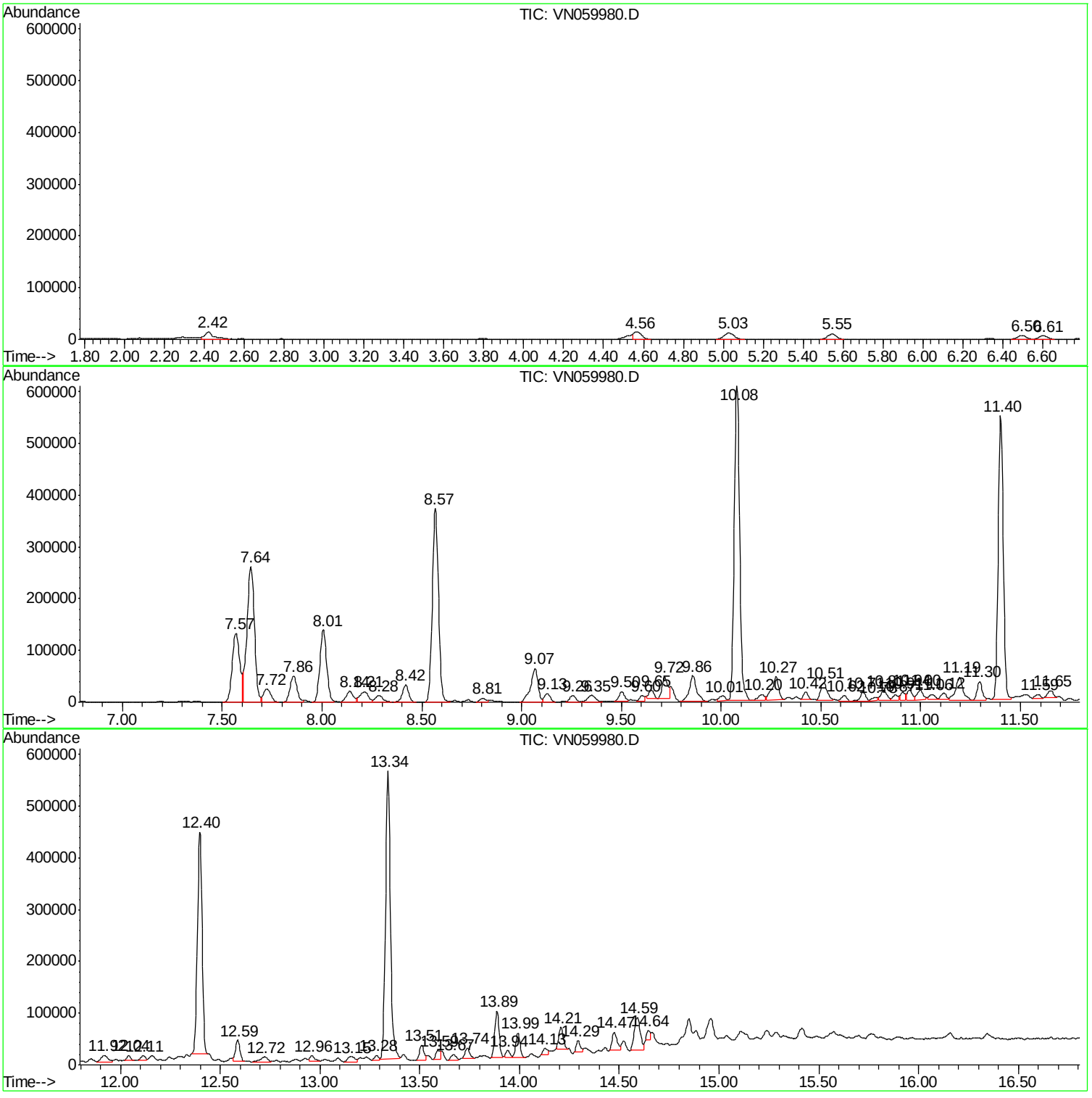
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : PD-3-(35-37)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N011320W.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\VN020320\
Data File : VN059980.D
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Instrument : MSVOA_N
ClientSampleId : PD-3-(35-37)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N011320W.M
Quant Title : SW846 8260

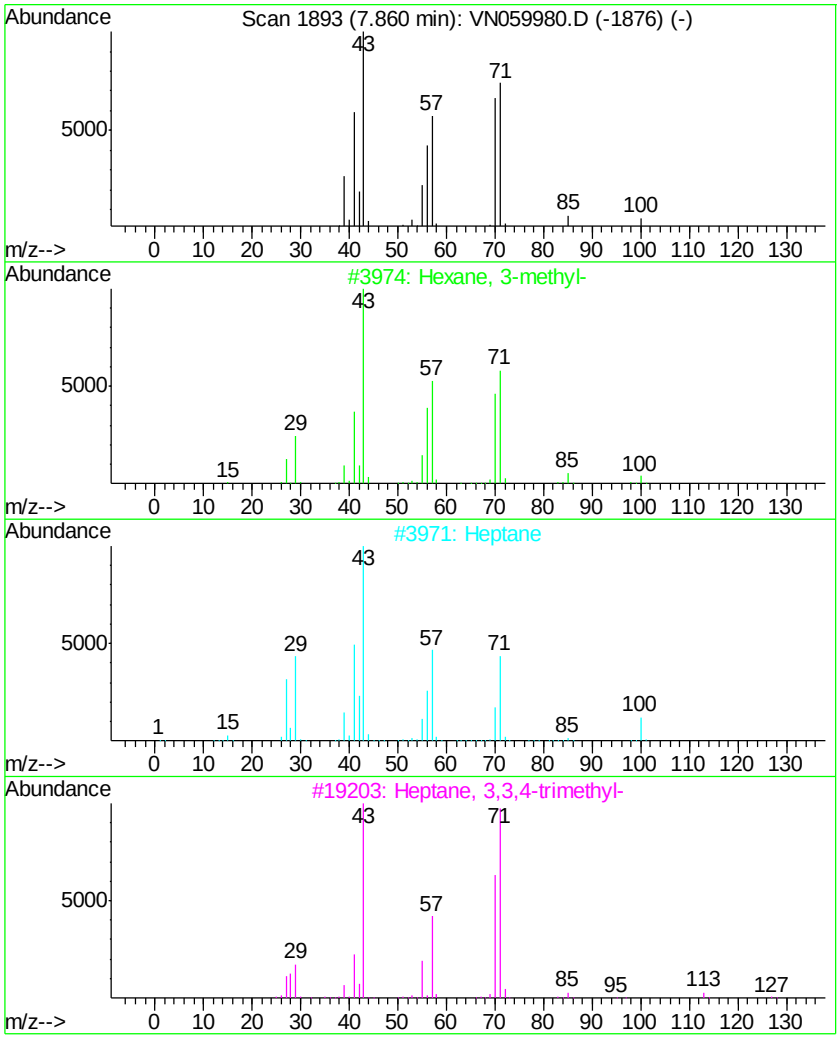
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

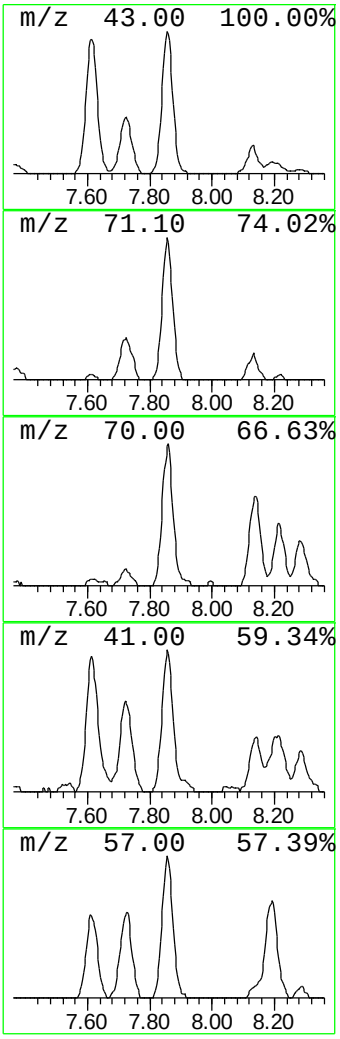
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.86	9.21 ug/l	124128	Pentafluorobenzene	7.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 3-methyl-	100	C7H16	000589-34-4	91
2	Heptane	100	C7H16	000142-82-5	80
3	Heptane, 3,3,4-trimethyl-	142	C10H22	020278-87-9	59
4	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	59
5	Pentane, 3-ethyl-	100	C7H16	000617-78-7	53





Library Search Compound Report

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Misc : 6.46g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : PD-3-(35-37)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N011320W.M
Quant Title : SW846 8260

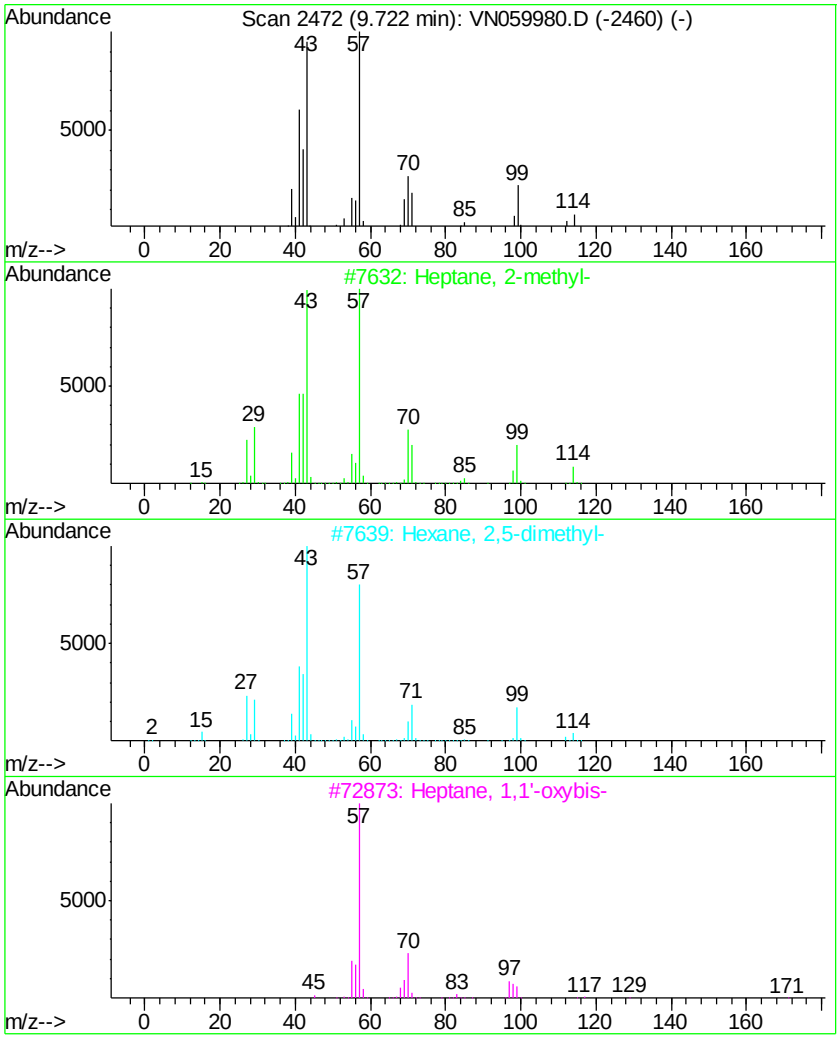
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

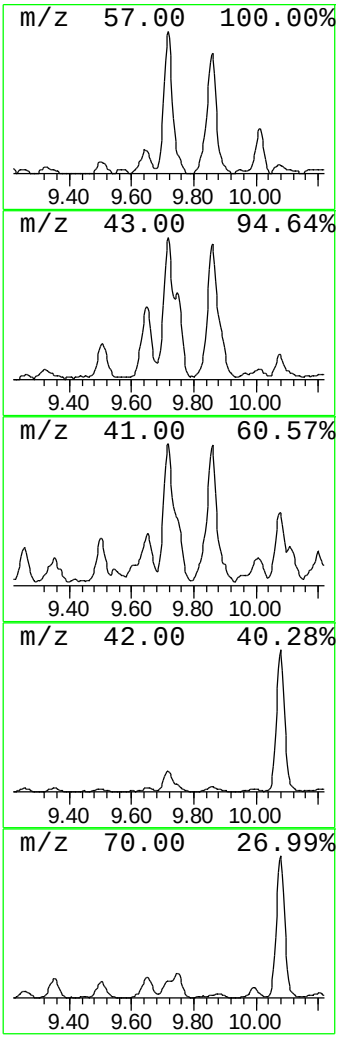
****

Peak Number 2 Heptane, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.72	5.22 ug/l	83095	1,4-Difluorobenzene	8.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane, 2-methyl-	114	C8H18	000592-27-8	93
2	Hexane, 2,5-dimethyl-	114	C8H18	000592-13-2	64
3	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	47
4	Cyclohexanol, 4-methyl-, cis-	114	C7H14O	007731-28-4	35
5	1-Pyrrolidinecarboxaldehyde	99	C5H9NO	003760-54-1	35





Library Search Compound Report

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Sample : L1346-05 20X
Misc : 6.46g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : PD-3-(35-37)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N011320W.M
Quant Title : SW846 8260

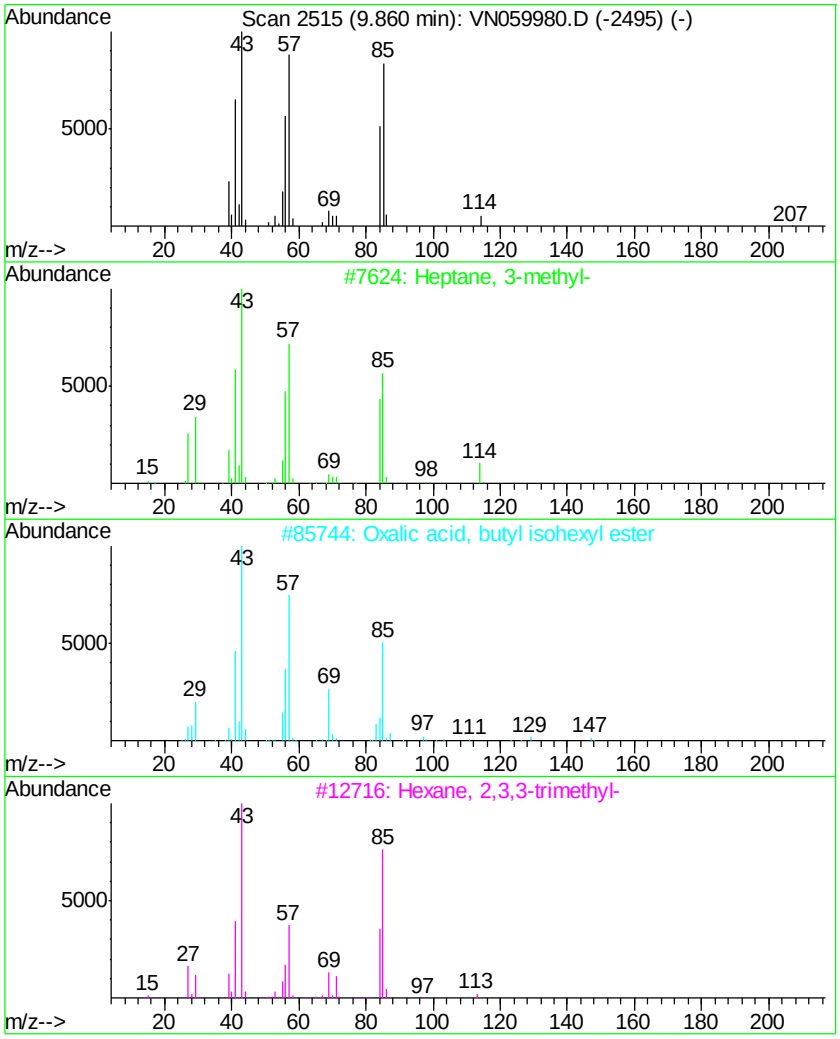
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

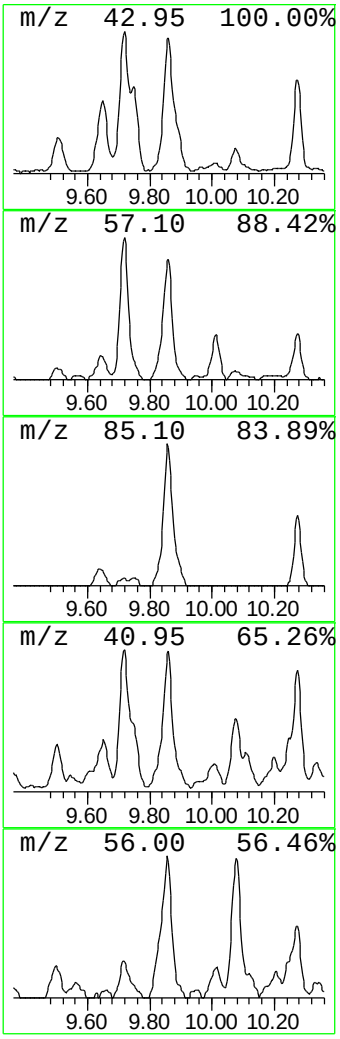
****

Peak Number 3 Heptane, 3-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.86	7.99 ug/l	127191	1,4-Difluorobenzene	8.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane, 3-methyl-	114	C8H18	000589-81-1	94
2	Oxalic acid, butyl isohexyl ester	230	C12H22O4	1000309-32-7	64
3	Hexane, 2,3,3-trimethyl-	128	C9H20	016747-28-7	59
4	Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	53
5	Pentane, 3-ethyl-2,4-dimethyl-	128	C9H20	001068-87-7	53





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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N011320W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
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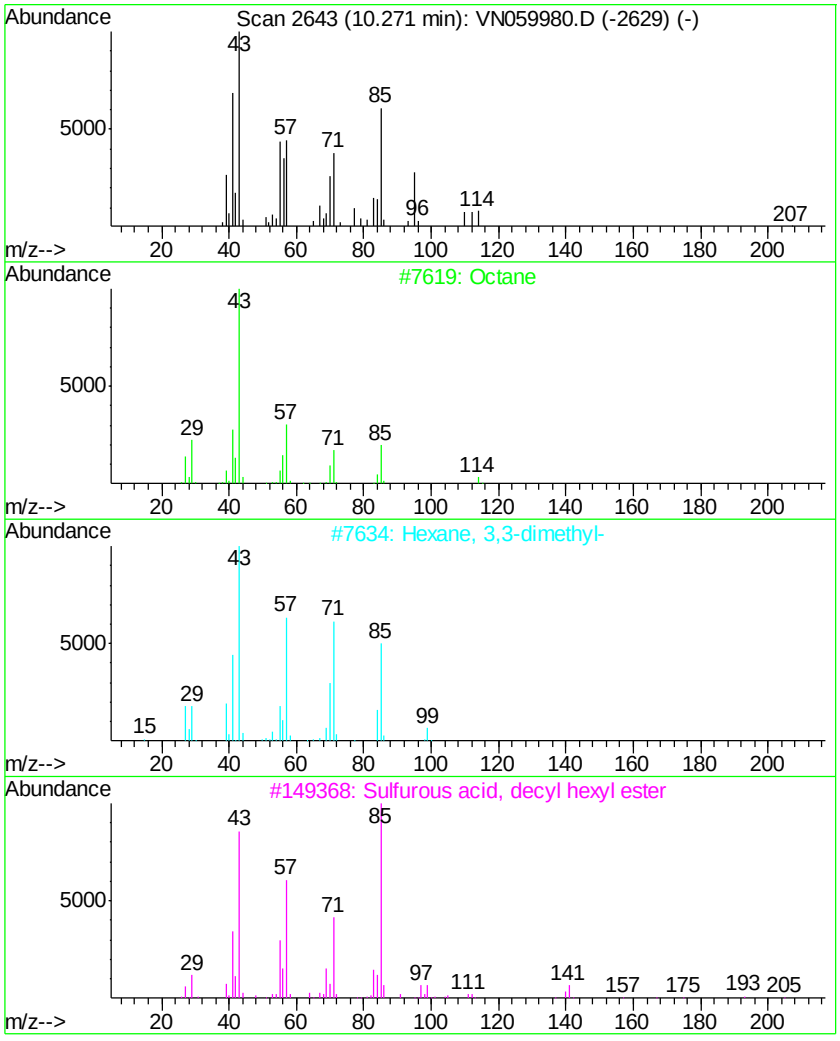
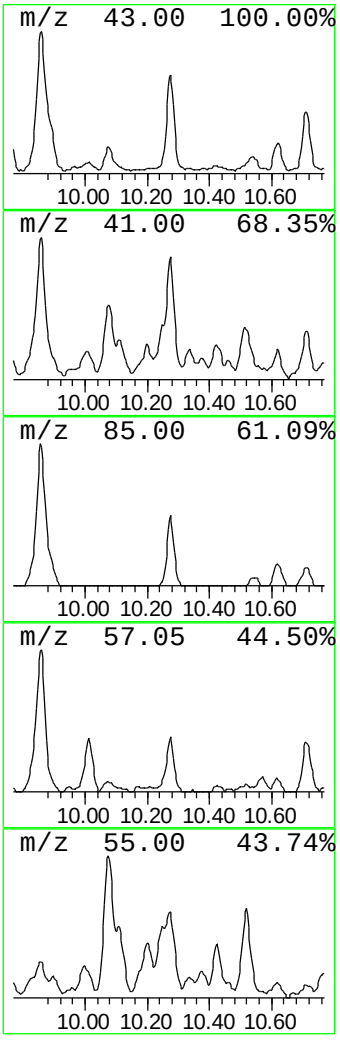
Peak Number 4 Octane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.27	5.60 ug/l	106333	Chlorobenzene-d5	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane	114	C8H18	000111-65-9	64
2	Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	50
3	Sulfurous acid, decyl hexyl ester	306	C16H34O3S	1000309-13-2	47
4	Sulfurous acid, dodecyl hexyl ester	334	C18H38O3S	1000309-13-4	47
5	Undecane, 2,4-dimethyl-	184	C13H28	017312-80-0	43





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Instrument : MSVOA_N
ClientSampleId : PD-3-(35-37)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N011320W.M
Quant Title : SW846 8260

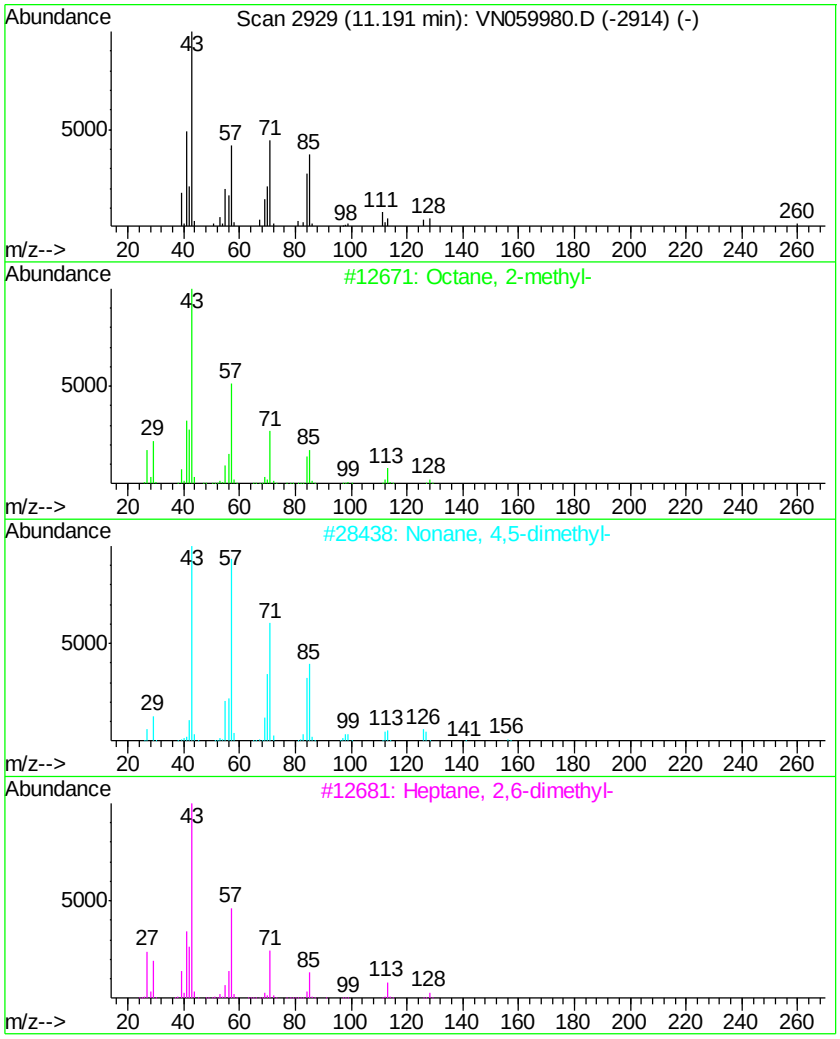
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

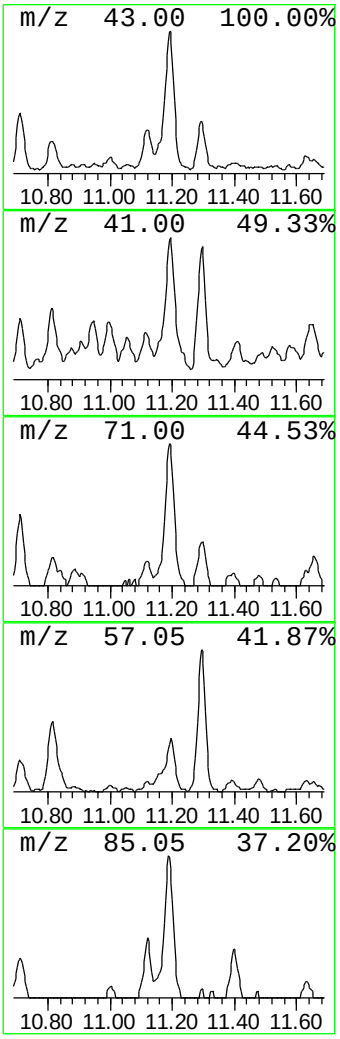
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.19	6.26 ug/l	118757	Chlorobenzene-d5	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2-methyl-	128	C9H20	003221-61-2	74
2	Nonane, 4,5-dimethyl-	156	C11H24	017302-23-7	53
3	Heptane, 2,6-dimethyl-	128	C9H20	001072-05-5	53
4	Pentane, 3-ethyl-2-methyl-	114	C8H18	000609-26-7	50
5	Dodecane, 5-methyl-	184	C13H28	017453-93-9	47





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ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : PD-3-(35-37)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N011320W.M
Quant Title : SW846 8260

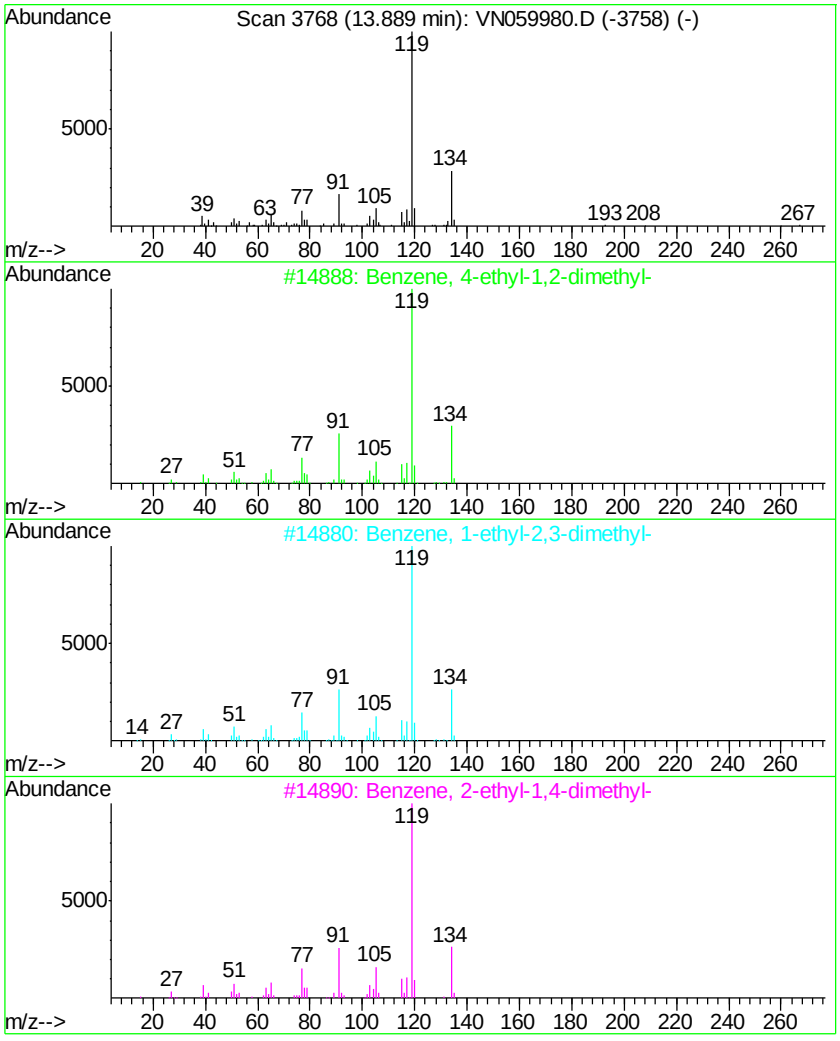
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

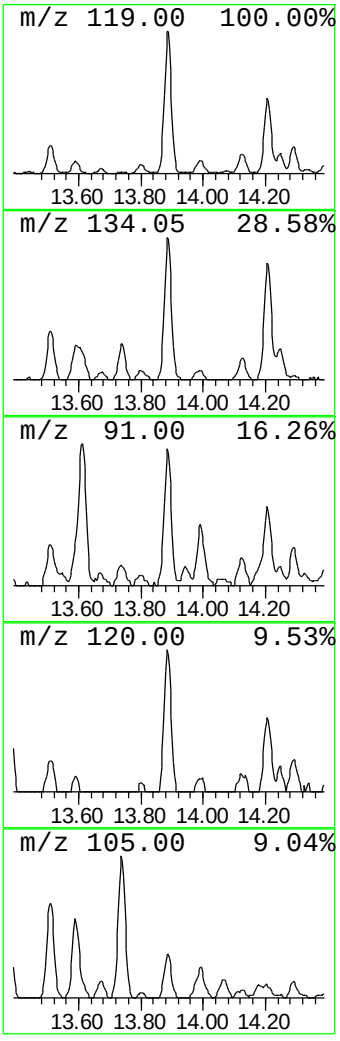
****

Peak Number 6 Benzene, 4-ethyl-1,2-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	7.28 ug/l	139597	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	96
2	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95
3	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	95
4	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	94
5	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	94





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Data File : VN059980.D
Acq On : 3 Feb 2020 17:19
Operator : JC/MD
Sample : L1346-05 20X
Misc : 6.46g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : PD-3-(35-37)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N011320W.M
Quant Title : SW846 8260

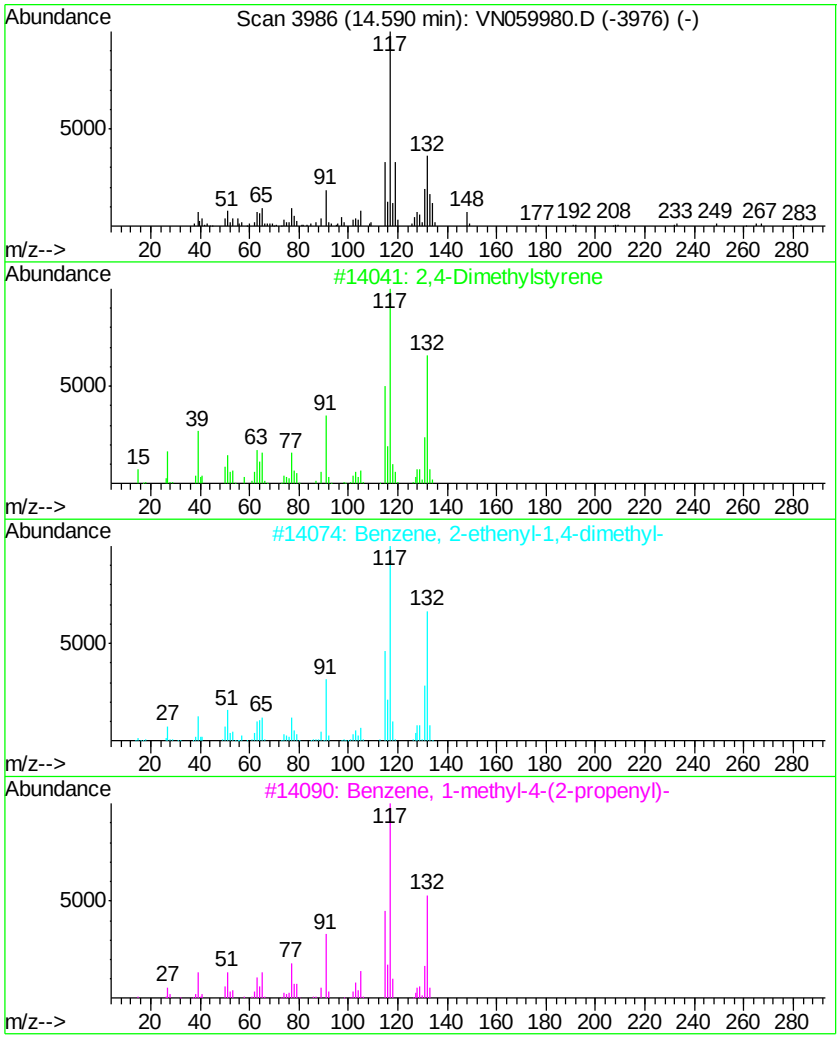
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

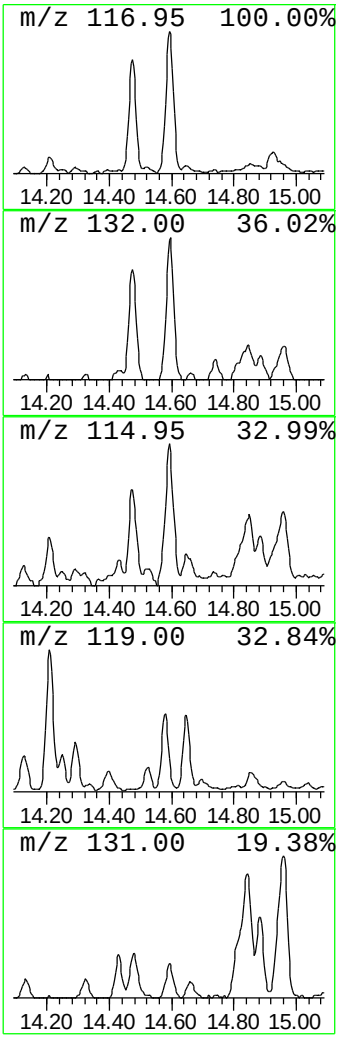
****

Peak Number 7 2,4-Dimethylstyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.59	6.87 ug/l	131889	1,4-Dichlorobenzene-d4	13.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4-Dimethylstyrene	132	C10H12	002234-20-0	92
2	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	91
3	Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	86
4	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000767-99-7	81
5	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	81





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN020320\
Data File : VN059980.D
Acq On : 3 Feb 2020 17:19
Operator : JC/MD
Sample : L1346-05 20X
Misc : 6.46g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : PD-3-(35-37)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N011320W.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-	7.86	9.2	ug/l	124128	1	7.64	673709	50.0
Heptane, 2-methyl-	9.72	5.2	ug/l	83095	2	8.57	796277	50.0
Heptane, 3-methyl-	9.86	8.0	ug/l	127191	2	8.57	796277	50.0
Octane	10.27	5.6	ug/l	106333	3	11.40	948777	50.0
Octane, 2-methyl-	11.19	6.3	ug/l	118757	3	11.40	948777	50.0
Benzene, 4-ethyl-...	13.89	7.3	ug/l	139597	4	13.34	959264	50.0
2,4-Dimethylstyrene	14.59	6.9	ug/l	131889	4	13.34	959264	50.0