LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN061618\
Data File : VN049325.D
Acq On : 16 Jun 2018 22:03
Operator : MD\SY
Sample : J3562-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : W-18

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\82N061618W.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	1.658	3	21	42	rBV	4403444	6514218	24.95%	2.416%
2	1.989	113	124	140	rBV	189950	374327	1.43%	0.139%
3	2.802	362	377	398	rVB	3368911	6789217	26.01%	2.518%
4	3.133	466	480	501	rVB2	1217528	2570600	9.85%	0.953%
5	3.796	664	686	710	rBV4	128768	437657	1.68%	0.162%
6	4.529	892	914	919	rBV2	895136	2440983	9.35%	0.905%
7	5.053	1046	1077	1106	rBV	1884078	6736525	25.80%	2.499%
8	5.378	1160	1178	1200	rVB4	110263	355836	1.36%	0.132%
9	5.567	1213	1237	1260	rBV2	416734	1332374	5.10%	0.494%
10	5.927	1312	1349	1371	rBV2	539772	1802025	6.90%	0.668%
11	6.069	1371	1393	1417	rBV2	442905	1481928	5.68%	0.550%
12	6.374	1464	1488	1502	rBV3	483024	1613303	6.18%	0.598%
13	6.625	1545	1566	1585	rBV	3984983	12367957	47.37%	4.587%
14	7.210	1725	1748	1764	rVB2	173856	572327	2.19%	0.212%
15	7.326	1764	1784	1822	rBV2	695295	2483465	9.51%	0.921%
16	7.593	1843	1867	1873	rBV2	1289552	3500546	13.41%	1.298%
17	7.657	1874	1887	1904	rVB3	5228236	14379606	55.08%	5.334%
18	7.876	1941	1955	1963	rBV	278724	677976	2.60%	0.251%
19	7.934	1963	1973	1988	rVB2	463681	1155597	4.43%	0.429%
20	8.030	1988	2003	2028	rBV2	1329400	3672694	14.07%	1.362%
21	8.159	2029	2043	2055	rBV	1048564	2543958	9.74%	0.944%
22	8.236	2055	2067	2079	rVV4	1721312	4372222	16.75%	1.622%
23	8.304	2080	2088	2108	rVV2	810633	1947981	7.46%	0.723%
24	8.410	2112	2121	2153	rVB7	378647	1212722	4.65%	0.450%
25	8.586	2157	2176	2198	rBV3	4094608	10510290	40.26%	3.898%
26	8.747	2215	2226	2236	rVB	370514	670189	2.57%	0.249%
27	8.821	2236	2249	2261	rBV	1710659	3802178	14.56%	1.410%
28	9.082	2303	2330	2347	rBV	4132863	10371729	39.73%	3.847%
29	9.271	2378	2389	2402	rVB2	436380	878139	3.36%	0.326%
30	9.365	2406	2418	2430	rBV4	199128	493121	1.89%	0.183%
31	9.435	2431	2440	2444	rBV4	213700	364790	1.40%	0.135%
32	9.512	2458	2464	2476	rVB3	229034	415130	1.59%	0.154%
33	9.615	2483	2496	2506	rBV2	1279005	2410356	9.23%	0.894%
34	9.667	2507	2512	2523	rVB3	152661	275386	1.05%	0.102%

LSC Area Percent Report

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Acq On : 16 Jun 2018 22:03
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Sample : J3562-04
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : W-18

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\82N061618W.M
Title : SW846 8260

35	9.844	2555	2567	2580	rBV7	211759	547054	2.10%	0.203%
36	9.969	2596	2606	2615	rBV	479801	873695	3.35%	0.324%
37	10.091	2631	2644	2674	rBV	5705628	11619615	44.51%	4.310%
38	10.255	2687	2695	2702	rBV2	343013	631903	2.42%	0.234%
39	10.432	2741	2750	2762	rVB	605301	1107011	4.24%	0.411%
40	10.522	2766	2778	2795	rVB5	931157	2026429	7.76%	0.752%
41	10.628	2805	2811	2822	rVB4	151102	271788	1.04%	0.101%
42	10.918	2894	2901	2907	rBV2	255495	428305	1.64%	0.159%
43	10.953	2908	2912	2921	rVV	265502	399348	1.53%	0.148%
44	11.008	2922	2929	2939	rVB	234914	394907	1.51%	0.146%
45	11.410	3041	3054	3068	rBV	3871907	7214375	27.63%	2.676%
46	11.509	3075	3085	3103	rVB2	938358	2042141	7.82%	0.757%
47	11.622	3104	3120	3142	rBV	1229333	2934802	11.24%	1.089%
48	12.252	3304	3316	3337	rVB	3044199	4951973	18.97%	1.837%
49	12.403	3350	3363	3380	rBV	3501062	5949338	22.79%	2.207%
50	12.593	3409	3422	3434	rBV	3568927	5621402	21.53%	2.085%
51	12.689	3434	3452	3459	rVV	3311608	5483992	21.01%	2.034%
52	12.734	3459	3466	3480	rVB	4114660	6567731	25.16%	2.436%
53	12.892	3503	3515	3531	rVB	6794088	10992147	42.10%	4.077%
54	13.043	3549	3562	3576	rBV	16686214	26106756	100.00%	9.683%
55	13.168	3588	3601	3612	rVB3	239459	565005	2.16%	0.210%
56	13.236	3612	3622	3631	rBV	324076	496955	1.90%	0.184%
57	13.290	3631	3639	3645	rBV2	246226	363063	1.39%	0.135%
58	13.348	3645	3657	3660	rBV	3601467	5553337	21.27%	2.060%
59	13.377	3661	3666	3679	rVB	5329468	8037084	30.79%	2.981%
60	13.516	3697	3709	3711	rBV2	884004	1187595	4.55%	0.440%
61	13.544	3711	3718	3726	rVV	2746697	4072421	15.60%	1.511%
62	13.589	3726	3732	3749	rVB4	1256421	2365736	9.06%	0.877%
63	13.676	3749	3759	3769	rVB2	218759	368779	1.41%	0.137%
64	13.744	3769	3780	3789	rBV	408471	648368	2.48%	0.240%
65	13.805	3789	3799	3804	rBV	1108520	1767937	6.77%	0.656%
66	13.892	3817	3826	3835	rBV	1594406	2339226	8.96%	0.868%
67	13.950	3835	3844	3850	rVV	1062831	1657020	6.35%	0.615%
68	13.998	3850	3859	3872	rVB	4002204	6358805	24.36%	2.359%
69	14.130	3889	3900	3912	rBV2	891365	1416682	5.43%	0.525%
70	14.213	3912	3926	3931	rBV	1475101	2367703	9.07%	0.878%
71	14.252	3931	3938	3947	rVB	2314095	3559322	13.63%	1.320%

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ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : W-18

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
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Start Thrs: 0.2 Max Peaks: 100
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Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N061618W.M
Title : SW846 8260

72	14.432	3985	3994	3999	rBV	191718	289429	1.11%	0.107%
73	14.477	3999	4008	4019	rVV	2398421	3877996	14.85%	1.438%
74	14.596	4031	4045	4057	rVV2	3895404	7173137	27.48%	2.661%
75	14.660	4057	4065	4076	rVB3	319258	547069	2.10%	0.203%
76	14.744	4081	4091	4105	rBV2	540675	922392	3.53%	0.342%
77	14.850	4106	4124	4131	rBV4	667021	1651829	6.33%	0.613%
78	14.962	4145	4159	4175	rVB2	873911	1993555	7.64%	0.739%
79	15.245	4238	4247	4255	rBV6	124194	274066	1.05%	0.102%
80	15.294	4257	4262	4281	rVB2	147422	269254	1.03%	0.100%
81	15.419	4290	4301	4314	rBV	257908	452177	1.73%	0.168%
82	15.583	4339	4352	4371	rBV2	153370	388888	1.49%	0.144%
83	15.776	4401	4412	4438	rVB4	112309	292058	1.12%	0.108%
84	16.165	4523	4533	4550	rVB2	148744	313434	1.20%	0.116%
85	16.358	4580	4593	4608	rBV2	152451	340028	1.30%	0.126%

Sum of corrected areas: 269602414

LSC Report - Integrated Chromatogram

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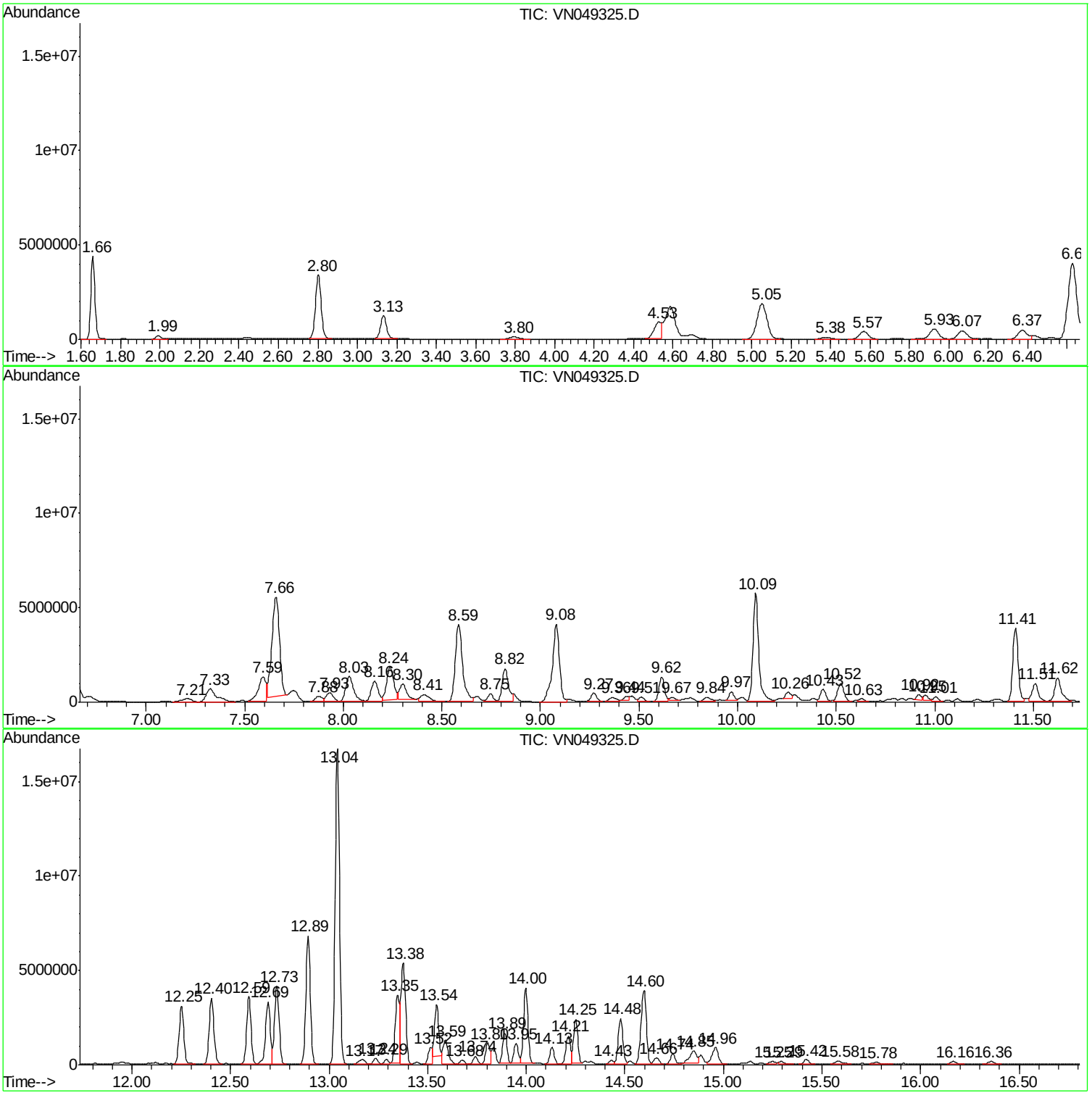
Acq On : 16 Jun 2018 22:03
Operator : MD\SY
Sample : J3562-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : W-18

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N061618W.M
Quant Title : SW846 8260

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



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN061618\
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Instrument : MSVOA_N
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N061618W.M
Quant Title : SW846 8260

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

****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.80	23.61 ug/l	6789220	Pentafluorobenzene	7.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	94
2	Pentane	72	C5H12	000109-66-0	36
3	3-Buten-1-ol	72	C4H8O	000627-27-0	28
4	Cyclobutane	56	C4H8	000287-23-0	9
5	Methane, isocyanato-	57	C2H3NO	000624-83-9	9

****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	23.42 ug/l	6736530	Pentafluorobenzene	7.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 3-methyl-	86	C6H14	000096-14-0	91
2	Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	78
3	Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	64
4	Pentane, 2,2,3-trimethyl-	114	C8H18	000564-02-3	50
5	Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	42

****

Peak Number 3 Cyclopentane, methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	43.01 ug/l	12368000	Pentafluorobenzene	7.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
3	Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
4	Cyclohexane	84	C6H12	000110-82-7	47
5	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	46

****

Peak Number 4 Benzene, 1-ethyl-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.

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Acq On : 16 Jun 2018 22:03
Operator : MD\SY
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Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : W-18

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N061618W.M
Quant Title : SW846 8260

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

12.89	98.97 ug/l	10992100	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	93
2	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90
3	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90
4	Mesitylene	120	C9H12	000108-67-8	90
5	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	90

****

Peak Number 5 Benzene, 1,1'-(1,5-hexadien... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.54	36.67 ug/l	4072420	1,4-Dichlorobenzene-d4	13.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,1'-(1,5-hexadiene-1,6...	234	C18H18	004439-45-6	53
2	Indole	117	C8H7N	000120-72-9	46
3	Benzyl nitrile	117	C8H7N	000140-29-4	43
4	Benzene, (2-bromocyclopropyl)-	196	C9H9Br	036617-02-4	42
5	Benzaldehyde, 4-(1-phenyl-2-prop...	238	C16H14O2	1000277-56-1	42

****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.00	57.25 ug/l	6358810	1,4-Dichlorobenzene-d4	13.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indan, 1-methyl-	132	C10H12	000767-58-8	93
2	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	87
3	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	87
4	Benzene, (2-methylcyclopropyl)-	132	C10H12	1000327-39-0	87
5	Benzene, (2-methyl-2-propenyl)-	132	C10H12	003290-53-7	86

****

Peak Number 7 Benzene, 1,2,3,5-tetramethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.25	32.05 ug/l	3559320	1,4-Dichlorobenzene-d4	13.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual

Library Search Compound Report

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Sample : J3562-04
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ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : W-18

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N061618W.M
Quant Title : SW846 8260

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

1	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	97
2	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	97
3	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	95
4	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	94
5	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	94

****

Peak Number 8 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.48	34.92 ug/l	3878000	1,4-Dichlorobenzene-d4	13.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	96
2	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	91
3	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	91
4	3-Phenylbut-1-ene	132	C10H12	000934-10-1	90
5	Indan, 1-methyl-	132	C10H12	000767-58-8	87

Tentatively Identified Compound (LSC) summary

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Instrument : MSVOA_N
ClientSampleId : W-18

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N061618W.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
Butane, 2-methyl-	2.80	23.6	ug/l	6789220	1	7.67	14379600	50.0
Pentane, 3-methyl-	5.05	23.4	ug/l	6736530	1	7.67	14379600	50.0
Cyclopentane, met...	6.63	43.0	ug/l	12368000	1	7.67	14379600	50.0
Benzene, 1-ethyl-...	12.89	99.0	ug/l	10992100	4	13.35	5553340	50.0
Benzene, 1,1'-(1,...	13.54	36.7	ug/l	4072420	4	13.35	5553340	50.0
Indan, 1-methyl-	14.00	57.3	ug/l	6358810	4	13.35	5553340	50.0
Benzene, 1,2,3,5-...	14.25	32.0	ug/l	3559320	4	13.35	5553340	50.0
Benzene, 2-etheny...	14.48	34.9	ug/l	3878000	4	13.35	5553340	50.0