LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX061318\
Data File : VX002542.D
Acq On : 14 Jun 2018 07:08
Operator : JC/MD
Sample : J3413-10
Misc : 7.51g/5mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 45 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : P-9AR

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_X\METHOD\82X060418W.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	1.069	75	79	93	rBV	939453	1213297	7.54%	0.347%
2	5.665	826	833	859	rVB2	289817	1216139	7.56%	0.348%
3	6.336	934	943	953	rVB	321413	963521	5.99%	0.276%
4	6.860	1020	1029	1038	rBV	374725	971273	6.04%	0.278%
5	7.452	1113	1126	1137	rBV2	293862	746495	4.64%	0.214%
6	8.055	1214	1225	1235	rVB	496124	1129788	7.02%	0.323%
7	8.177	1236	1245	1253	rBV	602633	1309555	8.14%	0.375%
8	8.500	1293	1298	1302	rBV	520542	815396	5.07%	0.233%
9	8.677	1319	1327	1330	rBV2	587163	1313027	8.16%	0.376%
10	8.720	1330	1334	1341	rVB	941062	1588596	9.88%	0.455%
11	9.561	1467	1472	1478	rBV2	488080	1056938	6.57%	0.303%
12	9.878	1519	1524	1529	rBV2	343013	799636	4.97%	0.229%
13	9.963	1534	1538	1543	rVB	1129805	1603043	9.97%	0.459%
14	10.067	1548	1555	1559	rBV	1094091	1527870	9.50%	0.437%
15	10.116	1559	1563	1568	rBV	813711	1187434	7.38%	0.340%
16	10.256	1580	1586	1591	rVB	1766791	2457387	15.28%	0.703%
17	10.366	1601	1604	1609	rVV2	1151746	1876759	11.67%	0.537%
18	10.415	1609	1612	1623	rVB	1476556	2223888	13.83%	0.637%
19	10.646	1643	1650	1654	rBV3	729789	1235387	7.68%	0.354%
20	10.835	1673	1681	1685	rBV2	1215858	1990870	12.38%	0.570%
21	10.914	1685	1694	1698	rBV3	1189651	2089363	12.99%	0.598%
22	11.024	1705	1712	1715	rBV2	519839	872198	5.42%	0.250%
23	11.140	1725	1731	1742	rVB6	1838081	4299100	26.73%	1.231%
24	11.250	1742	1749	1751	rBV	987998	1474063	9.16%	0.422%
25	11.280	1751	1754	1758	rVB4	771566	992490	6.17%	0.284%
26	11.366	1764	1768	1771	rBV	1374652	1709867	10.63%	0.489%
27	11.457	1777	1783	1786	rVV	1981204	3177077	19.75%	0.910%
28	11.512	1786	1792	1794	rVV2	3481977	5576203	34.67%	1.596%
29	11.536	1794	1796	1801	rVB2	3539110	3746073	23.29%	1.072%
30	11.677	1814	1819	1826	rVB	2263652	3613606	22.46%	1.034%
31	11.774	1832	1835	1837	rBV	1204920	1225598	7.62%	0.351%
32	11.817	1837	1842	1851	rVB	11905028	16085600	100.00%	4.605%
33	11.951	1857	1864	1868	rBV3	1138694	1921407	11.94%	0.550%
34	12.006	1868	1873	1875	rBV	1646790	2203361	13.70%	0.631%

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Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
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Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X060418W.M
Title : SW846 8260

35	12.030	1875	1877	1881	rVB2	1070037	1193173	7.42%	0.342%
36	12.085	1881	1886	1891	rBV3	1442905	2647432	16.46%	0.758%
37	12.152	1891	1897	1902	rBV3	2255719	3846493	23.91%	1.101%
38	12.231	1905	1910	1917	rVB3	1124081	2266743	14.09%	0.649%
39	12.304	1917	1922	1924	rBV2	3254394	4285348	26.64%	1.227%
40	12.329	1924	1926	1929	rVB	2371319	2404255	14.95%	0.688%
41	12.378	1929	1934	1940	rVB4	5950407	9605124	59.71%	2.750%
42	12.481	1944	1951	1955	rBV2	3227719	4437188	27.58%	1.270%
43	12.524	1955	1958	1964	rVB2	2654969	3784639	23.53%	1.083%
44	12.591	1964	1969	1971	rBV	2760834	3653018	22.71%	1.046%
45	12.615	1971	1973	1979	rVB	2849235	3083089	19.17%	0.883%
46	12.676	1979	1983	1986	rVB	3452498	3908913	24.30%	1.119%
47	12.762	1991	1997	1999	rBV2	1958720	3296351	20.49%	0.944%
48	12.859	2010	2013	2014	rVV2	834939	1003772	6.24%	0.287%
49	12.884	2014	2017	2019	rVV	1734561	2350341	14.61%	0.673%
50	12.908	2019	2021	2024	rVB2	1063409	1125888	7.00%	0.322%
51	12.951	2024	2028	2030	rBV2	1867910	2738262	17.02%	0.784%
52	12.981	2030	2033	2037	rVV	2688255	3709043	23.06%	1.062%
53	13.024	2037	2040	2047	rVB2	4046723	6946804	43.19%	1.989%
54	13.103	2047	2053	2056	rBV4	1739124	3513756	21.84%	1.006%
55	13.225	2066	2073	2077	rBV4	2542504	4552621	28.30%	1.303%
56	13.274	2077	2081	2084	rVB3	1503664	1584356	9.85%	0.454%
57	13.316	2084	2088	2091	rBV3	1873358	3244447	20.17%	0.929%
58	13.353	2091	2094	2099	rVV2	6280761	9084440	56.48%	2.601%
59	13.432	2104	2107	2112	rVV2	1145513	1775250	11.04%	0.508%
60	13.487	2112	2116	2124	rVB4	3738125	7433553	46.21%	2.128%
61	13.566	2125	2129	2132	rBV2	1538331	2232816	13.88%	0.639%
62	13.609	2132	2136	2138	rBV	1517037	1922105	11.95%	0.550%
63	13.646	2138	2142	2147	rBV3	2352300	3920365	24.37%	1.122%
64	13.731	2153	2156	2161	rVB2	2020770	2863605	17.80%	0.820%
65	13.841	2170	2174	2180	rVB	2842496	4351064	27.05%	1.246%
66	13.914	2180	2186	2191	rVB3	3171878	6522085	40.55%	1.867%
67	13.987	2191	2198	2203	rBV4	3455576	6869856	42.71%	1.967%
68	14.036	2203	2206	2209	rBV3	851367	1061820	6.60%	0.304%
69	14.066	2209	2211	2214	rVV	803939	1152255	7.16%	0.330%
70	14.140	2218	2223	2226	rBV3	3091760	4234452	26.32%	1.212%
71	14.225	2235	2237	2241	rVV	929392	999693	6.21%	0.286%

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ClientSampleId : P-9AR

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
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Title : SW846 8260

72	14.292	2242	2248	2254	rVB4	5620188	11106883	69.05%	3.180%
73	14.383	2259	2263	2268	rBV2	2208572	3061641	19.03%	0.876%
74	14.438	2268	2272	2276	rVB	3123056	3544495	22.04%	1.015%
75	14.481	2276	2279	2285	rVB6	1437643	2692074	16.74%	0.771%
76	14.548	2285	2290	2298	rBV3	3770591	7400543	46.01%	2.119%
77	14.621	2298	2302	2303	rBV3	732785	932709	5.80%	0.267%
78	14.682	2308	2312	2313	rBV2	6196727	7212063	44.84%	2.065%
79	14.706	2313	2316	2319	rVV	12297035	15356007	95.46%	4.396%
80	14.737	2319	2321	2326	rVB2	3359429	4091929	25.44%	1.171%
81	14.792	2326	2330	2333	rBV3	2106386	2994796	18.62%	0.857%
82	14.847	2335	2339	2343	rVV	8208154	10529514	65.46%	3.014%
83	14.883	2343	2345	2347	rVV2	1339789	1470750	9.14%	0.421%
84	14.914	2347	2350	2356	rVB3	2010852	2352903	14.63%	0.674%
85	14.969	2356	2359	2366	rBV2	1010900	1739633	10.81%	0.498%
86	15.115	2378	2383	2387	rBV3	1072641	1919533	11.93%	0.550%
87	15.255	2401	2406	2409	rBV	3138983	5416208	33.67%	1.551%
88	15.322	2414	2417	2419	rBV2	553529	803229	4.99%	0.230%
89	15.456	2434	2439	2442	rBV	4015157	6000402	37.30%	1.718%
90	15.487	2442	2444	2449	rVV3	1007371	1566721	9.74%	0.449%
91	15.560	2450	2456	2461	rVB	8101351	12335518	76.69%	3.531%
92	15.700	2473	2479	2482	rBV	7623391	12250925	76.16%	3.507%
93	15.737	2482	2485	2493	rVB	5219948	7859631	48.86%	2.250%
94	15.926	2508	2516	2531	rVB2	2076317	6288121	39.09%	1.800%
95	16.078	2537	2541	2546	rBV	1136665	1815721	11.29%	0.520%
96	16.182	2553	2558	2564	rBV	991464	1690087	10.51%	0.484%
97	16.285	2572	2575	2582	rVB2	751939	1318405	8.20%	0.377%
98	16.450	2597	2602	2610	rVB	1386924	2560215	15.92%	0.733%
99	16.700	2639	2643	2648	rVB	977541	1749750	10.88%	0.501%
100	16.761	2648	2653	2657	rBV	881627	1434432	8.92%	0.411%

Sum of corrected areas: 349311558

LSC Report - Integrated Chromatogram

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Operator : JC/MD
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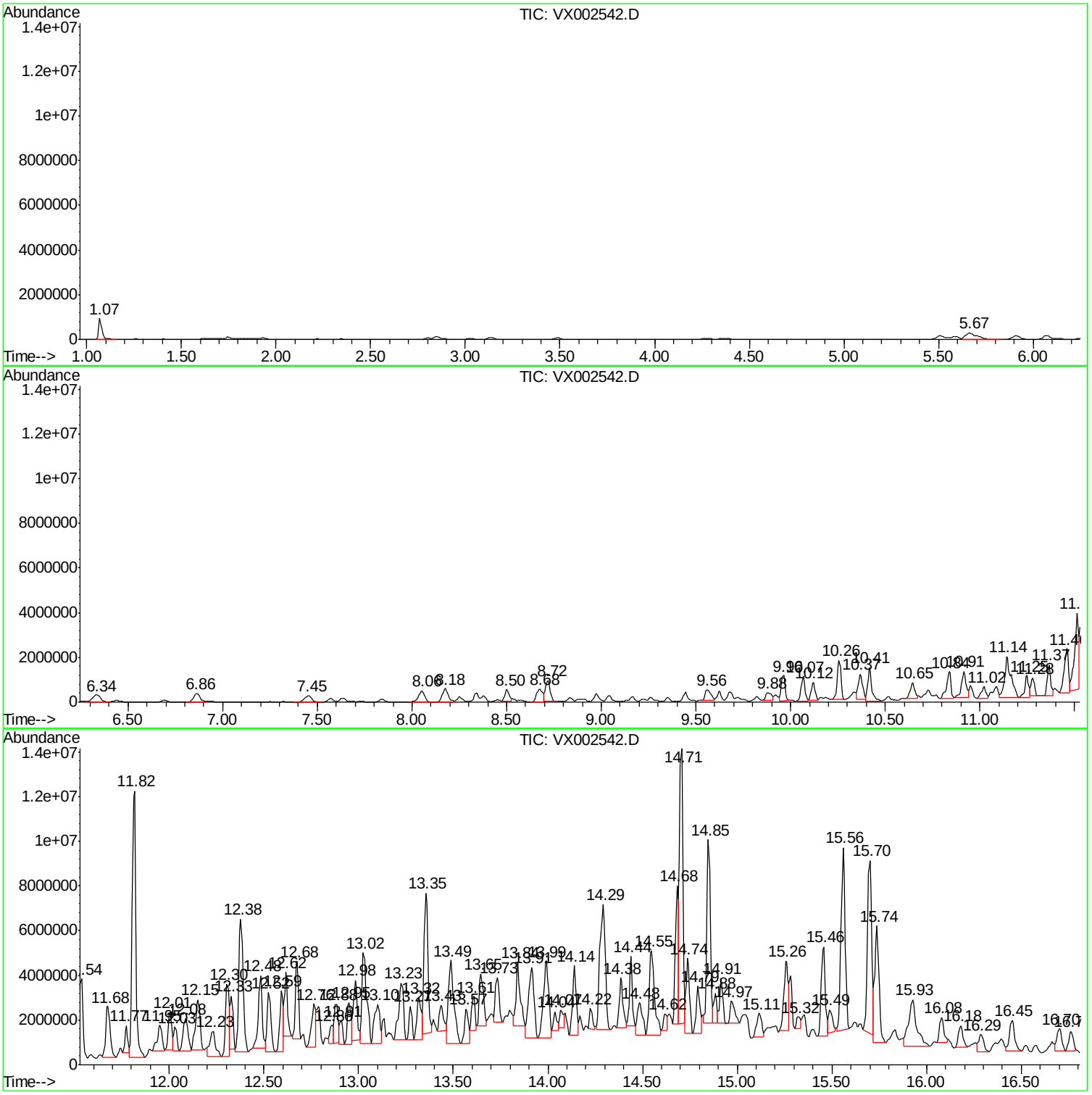
Misc : 7.51g/5mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 45 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : P-9AR

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X060418W.M
Quant Title : SW846 8260

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



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Quant Title : SW846 8260

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

****

Peak Number 1 Benzene, 1-ethyl-3,5-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.38	181.41 ug/l	9605120	1,4-Dichlorobenzene-d4	12.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	95
2	o-Cymene	134	C10H14	000527-84-4	94
3	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	93
4	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	93
5	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	93

****

Peak Number 2 Benzene, 2-butenyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.35	171.57 ug/l	9084440	1,4-Dichlorobenzene-d4	12.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-butenyl-	132	C10H12	001560-06-1	89
2	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	86
3	1-Phenyl-1-butene	132	C10H12	000824-90-8	86
4	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	70
5	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000767-99-7	70

****

Peak Number 3 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.49	140.39 ug/l	7433550	1,4-Dichlorobenzene-d4	12.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-	132	C10H12	000119-64-2	89
2	2H-Inden-2-one, 1,3-dihydro-	132	C9H8O	000615-13-4	43
3	Benzene, cyclobutyl-	132	C10H12	004392-30-7	38
4	2-Methylbenzyl alcohol, pentaflu...	268	C11H9F5O2	1000364-54-1	35
5	2-Methylbenzyl cyanide	131	C9H9N	022364-68-7	35

****

Peak Number 4 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 4

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

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Instrument : MSVOA_X
ClientSampleId : P-9AR

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X060418W.M
Quant Title : SW846 8260

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.29	209.77 ug/l	11106900	1,4-Dichlorobenzene-d4	12.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	95
2	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	95
3	Benzene, (1,2-dimethyl-1-propenyl)-	146	C11H14	000769-57-3	91
4	Benzene, (2-methyl-1-butenyl)-	146	C11H14	056253-64-6	70
5	1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	70

****

Peak Number 5 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.55	139.77 ug/l	7400540	1,4-Dichlorobenzene-d4	12.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	68
2	1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	53
3	2-Propenal, 3-(4-methylphenyl)-	146	C10H10O	001504-75-2	53
4	Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	53
5	Benzene, (1-methyl-1-butenyl)-	146	C11H14	053172-84-2	49

****

Peak Number 6 Naphthalene, 1-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.71	290.02 ug/l	15356000	1,4-Dichlorobenzene-d4	12.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	94
2	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	94
3	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
4	Benzocycloheptatriene	142	C11H10	000264-09-5	59
5	Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	45

****

Peak Number 7 Naphthalene, 2,6-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.56	232.97 ug/l	12335500	1,4-Dichlorobenzene-d4	12.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual

Library Search Compound Report

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Instrument : MSVOA_X
ClientSampleId : P-9AR

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X060418W.M
Quant Title : SW846 8260

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

1	Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	97
2	Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	96
3	Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	96
4	Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	96
5	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	96

****

Peak Number 8 Naphthalene, 2,3-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.70	231.37 ug/l	12250900	1,4-Dichlorobenzene-d4	12.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	97
2	Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	97
3	Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	97
4	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	97
5	Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	97

Tentatively Identified Compound (LSC) summary

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ClientSampleId : P-9AR

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X060418W.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
Benzene, 1-ethyl-...	12.38	181.4	ug/l	9605120	4	12.09	2647430	50.0
Benzene, 2-butenyl-	13.35	171.6	ug/l	9084440	4	12.09	2647430	50.0
Naphthalene, 1,2,...	13.49	140.4	ug/l	7433550	4	12.09	2647430	50.0
Naphthalene, 1,2,...	14.29	209.8	ug/l	11106900	4	12.09	2647430	50.0
Naphthalene, 1,2,...	14.55	139.8	ug/l	7400540	4	12.09	2647430	50.0
Naphthalene, 1-me...	14.71	290.0	ug/l	15356000	4	12.09	2647430	50.0
Naphthalene, 2,6-...	15.56	233.0	ug/l	12335500	4	12.09	2647430	50.0
Naphthalene, 2,3-...	15.70	231.4	ug/l	12250900	4	12.09	2647430	50.0