LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX032419\
Data File : VX008403.D
Acq On : 24 Mar 2019 19:34
Operator : JC/SP
Sample : K2059-05
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-2

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\82X032319W.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	1.276	15	20	23	rBV	532648	701371	12.48%	0.941%
2	1.404	38	41	47	rBV	319757	307193	5.47%	0.412%
3	1.788	99	104	120	rVB	4013920	5620062	100.00%	7.544%
4	2.001	133	139	152	rVB	1627011	2410978	42.90%	3.236%
5	2.263	176	182	194	rVB	448508	723167	12.87%	0.971%
6	2.391	194	203	217	rVB	286370	605636	10.78%	0.813%
7	2.849	254	278	280	rBV	683918	1519990	27.05%	2.040%
8	2.891	280	285	290	rVV	1437160	2571661	45.76%	3.452%
9	3.172	321	331	347	rBV	1475936	3443663	61.27%	4.623%
10	3.397	357	368	379	rVB	65411	155691	2.77%	0.209%
11	3.525	379	389	404	rBV	346740	796916	14.18%	1.070%
12	3.818	421	437	446	rBV	371460	920880	16.39%	1.236%
13	3.928	446	455	463	rVV	262058	712375	12.68%	0.956%
14	4.202	485	500	508	rVV2	247383	826410	14.70%	1.109%
15	4.312	512	518	524	rVV	111506	339165	6.03%	0.455%
16	4.403	524	533	545	rVV	1255318	3729747	66.36%	5.007%
17	4.531	545	554	570	rVB2	116027	379302	6.75%	0.509%
18	5.305	655	681	696	rVB5	171905	893131	15.89%	1.199%
19	5.501	696	713	719	rBV3	181911	622472	11.08%	0.836%
20	5.598	719	729	736	rBV5	411246	1659821	29.53%	2.228%
21	5.726	745	750	771	rVB3	379059	1370139	24.38%	1.839%
22	5.933	771	784	796	rBV2	505820	1525042	27.14%	2.047%
23	6.061	797	805	813	rVV	171109	444520	7.91%	0.597%
24	6.263	823	838	847	rVV4	299367	1428638	25.42%	1.918%
25	6.354	848	853	862	rVV3	362067	1049541	18.67%	1.409%
26	6.458	862	870	882	rVB2	310292	868847	15.46%	1.166%
27	6.702	897	910	923	rVB2	110790	307067	5.46%	0.412%
28	6.860	926	936	942	rBV	413099	1040899	18.52%	1.397%
29	6.939	942	949	961	rVB3	382621	1125078	20.02%	1.510%
30	7.067	961	970	976	rBV	85702	205564	3.66%	0.276%
31	7.153	976	984	993	rVB2	131196	300969	5.36%	0.404%
32	7.256	993	1001	1009	rBV	307346	662802	11.79%	0.890%
33	7.458	1022	1034	1046	rBV4	795596	2226582	39.62%	2.989%
34	7.573	1046	1053	1058	rVV2	42623	96372	1.71%	0.129%

LSC Area Percent Report

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Data File : VX008403.D
Acq On : 24 Mar 2019 19:34
Operator : JC/SP
Sample : K2059-05
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-2

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\82X032319W.M
Title : SW846 8260

35	7.634	1058	1063	1069	rVV	61441	136598	2.43%	0.183%
36	7.732	1073	1079	1092	rVV	211057	469768	8.36%	0.631%
37	7.848	1092	1098	1105	rVB2	75507	151293	2.69%	0.203%
38	7.957	1113	1116	1123	rVB2	160083	303178	5.39%	0.407%
39	8.055	1123	1132	1144	rVB2	112467	334510	5.95%	0.449%
40	8.177	1144	1152	1154	rBV2	224323	446460	7.94%	0.599%
41	8.213	1154	1158	1163	rVV	528233	922977	16.42%	1.239%
42	8.256	1163	1165	1174	rVB4	85084	150798	2.68%	0.202%
43	8.378	1176	1185	1190	rBV5	80292	176318	3.14%	0.237%
44	8.500	1200	1205	1209	rBV2	94075	153739	2.74%	0.206%
45	8.567	1209	1216	1226	rVB3	499171	930190	16.55%	1.249%
46	8.671	1226	1233	1235	rBV2	141150	246471	4.39%	0.331%
47	8.713	1235	1240	1247	rVV	906697	1456269	25.91%	1.955%
48	8.793	1247	1253	1257	rVV3	50954	118310	2.11%	0.159%
49	8.835	1257	1260	1264	rVV2	68868	109986	1.96%	0.148%
50	8.902	1264	1271	1277	rVV2	214307	497975	8.86%	0.668%
51	8.988	1280	1285	1289	rVV2	169791	329406	5.86%	0.442%
52	9.037	1289	1293	1299	rVV4	93336	191952	3.42%	0.258%
53	9.091	1299	1302	1306	rVV	64892	110987	1.97%	0.149%
54	9.165	1306	1314	1319	rVV	155863	352666	6.28%	0.473%
55	9.219	1319	1323	1335	rVB	328326	573158	10.20%	0.769%
56	9.500	1363	1369	1370	rBV2	94665	159205	2.83%	0.214%
57	9.567	1375	1380	1385	rVV3	117848	272811	4.85%	0.366%
58	9.622	1385	1389	1392	rVV	119515	174720	3.11%	0.235%
59	9.658	1392	1395	1401	rVV2	118126	183917	3.27%	0.247%
60	9.817	1415	1421	1428	rBV3	85964	152847	2.72%	0.205%
61	10.073	1458	1463	1465	rBV2	115800	170467	3.03%	0.229%
62	10.110	1465	1469	1474	rVV	779038	1042395	18.55%	1.399%
63	10.158	1474	1477	1480	rVV	140504	205984	3.67%	0.277%
64	10.201	1480	1484	1488	rVV2	255092	419876	7.47%	0.564%
65	10.250	1488	1492	1496	rVV	784518	1008453	17.94%	1.354%
66	10.298	1496	1500	1504	rVV	67098	149551	2.66%	0.201%
67	10.359	1505	1510	1515	rVV	380246	540022	9.61%	0.725%
68	10.475	1524	1529	1532	rVV2	61922	104357	1.86%	0.140%
69	10.634	1548	1555	1563	rBV4	53450	141782	2.52%	0.190%
70	11.018	1610	1618	1624	rBV	1227228	1568824	27.91%	2.106%
71	11.134	1633	1637	1642	rBV	634956	788438	14.03%	1.058%

LSC Area Percent Report

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Sample : K2059-05
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-2

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\82X032319W.M
Title : SW846 8260

72	11.323	1663	1668	1670	rBV	112665	149514	2.66%	0.201%
73	11.359	1670	1674	1682	rVB	857750	1065319	18.96%	1.430%
74	11.451	1683	1689	1693	rBV	260769	336223	5.98%	0.451%
75	11.506	1693	1698	1705	rVB	90085	155522	2.77%	0.209%
76	11.664	1715	1724	1733	rVB	673788	874279	15.56%	1.174%
77	11.945	1767	1770	1775	rVV	137663	189686	3.38%	0.255%
78	12.024	1779	1783	1786	rVV	77633	95866	1.71%	0.129%
79	12.073	1786	1791	1797	rVV	734058	1007469	17.93%	1.352%
80	12.140	1797	1802	1814	rVV	444333	604391	10.75%	0.811%
81	12.298	1822	1828	1835	rBV	3167439	3836413	68.26%	5.150%
82	12.365	1835	1839	1850	rVB2	303129	533245	9.49%	0.716%
83	12.457	1850	1854	1859	rVB	127165	155358	2.76%	0.209%
84	12.518	1859	1864	1870	rVB	415756	499191	8.88%	0.670%
85	12.585	1870	1875	1883	rVB	93481	115582	2.06%	0.155%
86	12.664	1883	1888	1892	rBV	1314951	1627277	28.95%	2.184%
87	12.700	1892	1894	1898	rVB	206624	211211	3.76%	0.284%
88	12.755	1898	1903	1910	rBV2	772602	1108727	19.73%	1.488%
89	12.975	1932	1939	1943	rBV	943107	1094966	19.48%	1.470%
90	13.078	1952	1956	1962	rBV3	75582	140173	2.49%	0.188%
91	13.225	1976	1980	1987	rVB	624498	749110	13.33%	1.006%
92	13.347	1995	2000	2005	rVB2	945421	1285371	22.87%	1.725%
93	13.481	2018	2022	2027	rVB	94893	123782	2.20%	0.166%
94	13.597	2038	2041	2044	rVV	134015	181493	3.23%	0.244%
95	13.633	2044	2047	2052	rVV3	157647	235907	4.20%	0.317%
96	13.719	2058	2061	2067	rVB2	139460	225533	4.01%	0.303%
97	13.834	2072	2080	2089	rBV	395918	533323	9.49%	0.716%
98	14.133	2124	2129	2133	rBV	85531	106741	1.90%	0.143%
99	14.273	2147	2152	2157	rBV	75882	126802	2.26%	0.170%
100	14.834	2240	2244	2254	rVB	212965	288546	5.13%	0.387%

Sum of corrected areas: 74495369

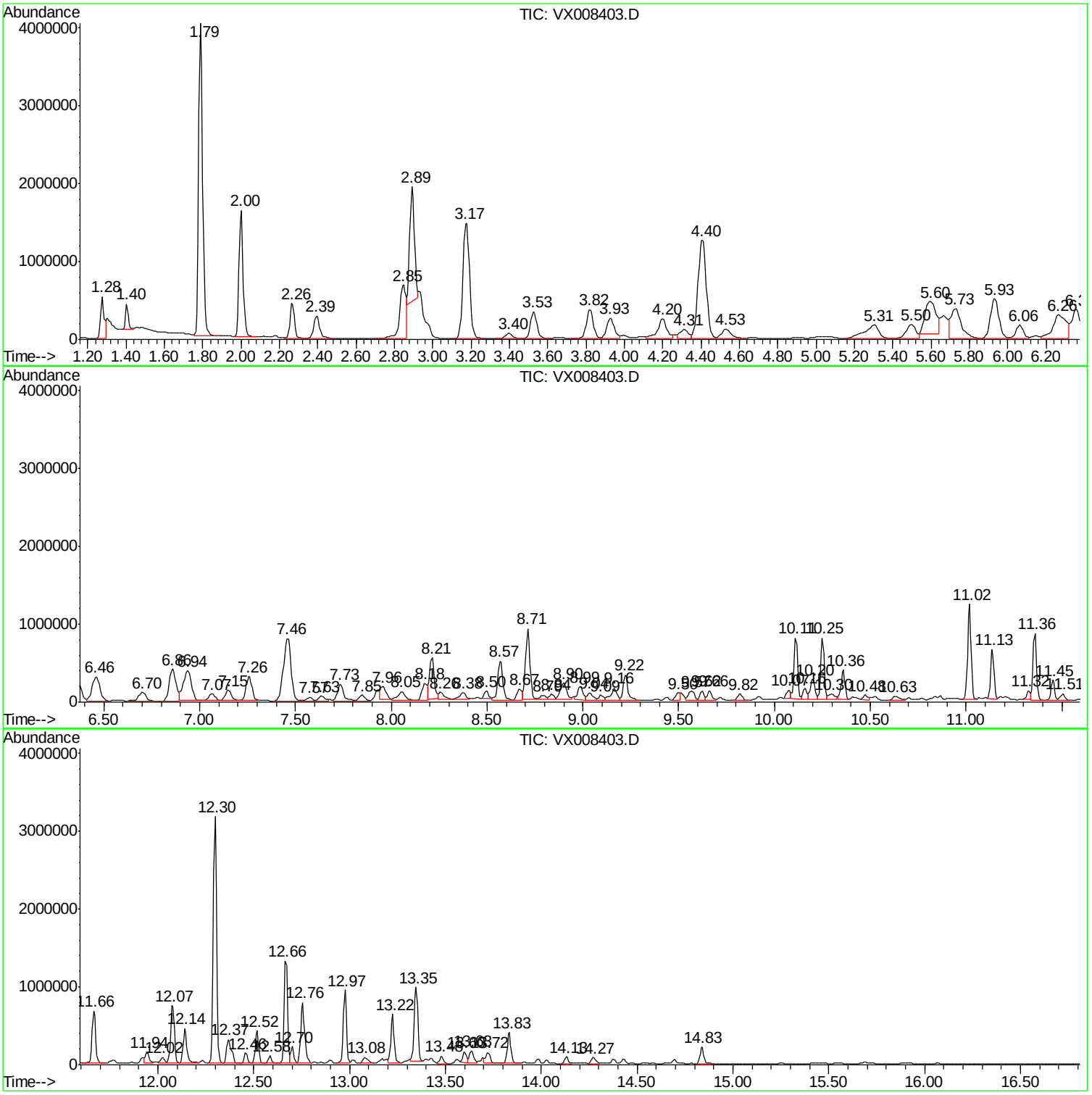
LSC Report - Integrated Chromatogram

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX032419\
Data File : VX008403.D
Acq On : 24 Mar 2019 19:34
Operator : JC/SP
Sample : K2059-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-2

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X032319W.M
Quant Title : SW846 8260

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



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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X032319W.M
Quant Title : SW846 8260

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

****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.79	205.09 ug/l	5620060	Pentafluorobenzene	5.67

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	25
4	1-Butene	56	C4H8	000106-98-9	10
5	Methane, isocyanato-	57	C2H3NO	000624-83-9	9

****

Peak Number 2 Pentane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.00	87.98 ug/l	2410980	Pentafluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane	72	C5H12	000109-66-0	91
2	Butane, 2-methyl-	72	C5H12	000078-78-4	38
3	Oxirane, ethyl-	72	C4H8O	000106-88-7	9
4	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	9
5	Butanal, 2,2-dimethyl-	100	C6H12O	002094-75-9	9

****

Peak Number 3 Butane, 2,3-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.85	55.47 ug/l	1519990	Pentafluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	86
2	Pentane, 2-methyl-	86	C6H14	000107-83-5	50
3	Pyrrolidine	71	C4H9N	000123-75-1	10
4	Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	9
5	Tetrahydrofuran	72	C4H8O	000109-99-9	9

****

Peak Number 4 Pentane, 2-methyl- Concentration Rank 5

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

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Acq On : 24 Mar 2019 19:34
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Sample : K2059-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-2

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X032319W.M
Quant Title : SW846 8260

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

2.89	93.85 ug/l	2571660	Pentafluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2-methyl-	86	C6H14	000107-83-5	91
2	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	43
3	Pentane	72	C5H12	000109-66-0	43
4	1-Butanol, 2,3-dimethyl-	102	C6H14O	019550-30-2	36
5	Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	28

****

Peak Number 5 Pentane, 3-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.17	125.67 ug/l	3443660	Pentafluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 3-methyl-	86	C6H14	000096-14-0	91
2	Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	45
3	3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	42
4	Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	40
5	Butyl isocyanatoacetate	157	C7H11NO3	017046-22-9	40

****

Peak Number 6 Cyclopentane, methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.40	136.11 ug/l	3729750	Pentafluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2	Cyclopropane, propyl-	84	C6H12	002415-72-7	78
3	Cyclobutane, ethyl-	84	C6H12	004806-61-5	72
4	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	64
5	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	50

****

Peak Number 7 Hexane, 3-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.93	55.65 ug/l	1525040	Pentafluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual

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Sample : K2059-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-2

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X032319W.M
Quant Title : SW846 8260

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

1	Hexane, 3-methyl-	100	C7H16	000589-34-4	91
2	Heptane	100	C7H16	000142-82-5	80
3	Heptane, 3,4-dimethyl-	128	C9H20	000922-28-1	59
4	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	53
5	Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	50

****

Peak Number 8 Indane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.30	190.40 ug/l	3836410	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	76
2	Benzene, 2-propenyl-	118	C9H10	000300-57-2	70
3	Benzene, cyclopropyl-	118	C9H10	000873-49-4	70
4	Deltacyclene	118	C9H10	007785-10-6	52
5	Benzene, 1-propenyl-	118	C9H10	000637-50-3	46

****

Peak Number 9 Benzene, 2-ethyl-1,4-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.66	80.76 ug/l	1627280	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	95
2	o-Cymene	134	C10H14	000527-84-4	95
3	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95
4	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	94
5	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	94

****

Peak Number 10 1-Phenyl-1-butene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.35	63.79 ug/l	1285370	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenyl-1-butene	132	C10H12	000824-90-8	86
2	3-Phenylbut-1-ene	132	C10H12	000934-10-1	70
3	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	70

Library Search Compound Report

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Sample : K2059-05
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Instrument :
MSVOA_X
ClientSampleId :
MW-2

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X032319W.M
Quant Title : SW846 8260

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

4	Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	70
5	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	70

Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX032419\
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X032319W.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-	1.79	205.1	ug/l	5620060	1	5.67	1370140	50.0
Pentane	2.00	88.0	ug/l	2410980	1	5.67	1370140	50.0
Butane, 2,3-dimet...	2.85	55.5	ug/l	1519990	1	5.67	1370140	50.0
Pentane, 2-methyl-	2.89	93.8	ug/l	2571660	1	5.67	1370140	50.0
Pentane, 3-methyl-	3.17	125.7	ug/l	3443660	1	5.67	1370140	50.0
Cyclopentane, met...	4.40	136.1	ug/l	3729750	1	5.67	1370140	50.0
Hexane, 3-methyl-	5.93	55.7	ug/l	1525040	1	5.67	1370140	50.0
Indane	12.30	190.4	ug/l	3836410	4	12.08	1007470	50.0
Benzene, 2-ethyl-...	12.66	80.8	ug/l	1627280	4	12.08	1007470	50.0
1-Phenyl-1-butene	13.35	63.8	ug/l	1285370	4	12.08	1007470	50.0