

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX082718\
 Data File : VX004262.D
 Acq On : 27 Aug 2018 14:21
 Operator : JC/MD
 Sample : J4646-14
 Misc : 5.27g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 EP1-Q4-D7

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\82X082218W.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	1119832	1397948	4.46%	0.325%
2	5.501	792	806	819	rBV	179767	510558	1.63%	0.119%
3	5.653	819	831	846	rVV	259579	721685	2.30%	0.168%
4	6.062	887	898	917	rBV	197043	512623	1.64%	0.119%
5	6.854	1017	1028	1043	rBV	407146	959462	3.06%	0.223%
6	8.714	1327	1333	1348	rVB	1019815	1578773	5.04%	0.367%
7	9.677	1485	1491	1495	rBV	395653	606188	1.94%	0.141%
8	9.890	1518	1526	1530	rBV3	428975	1037621	3.31%	0.241%
9	9.951	1533	1536	1542	rVB	431379	594225	1.90%	0.138%
10	10.061	1548	1554	1558	rBV	929142	1290691	4.12%	0.300%
11	10.116	1558	1563	1567	rVV	884305	1264504	4.04%	0.294%
12	10.238	1578	1583	1589	rBV3	331797	623064	1.99%	0.145%
13	10.335	1589	1599	1602	rBV	929061	1748112	5.58%	0.406%
14	10.378	1602	1606	1609	rVB	986326	1246213	3.98%	0.289%
15	10.409	1609	1611	1623	rVB4	733666	1418256	4.53%	0.329%
16	10.512	1623	1628	1634	rBV	799053	1205220	3.85%	0.280%
17	10.591	1636	1641	1643	rBV2	473389	749118	2.39%	0.174%
18	10.640	1643	1649	1654	rBV2	3158199	5331426	17.02%	1.238%
19	10.726	1657	1663	1667	rBV2	2345820	3699701	11.81%	0.859%
20	10.768	1667	1670	1673	rVB2	1337124	1643971	5.25%	0.382%
21	10.835	1673	1681	1685	rBV	9746246	14649738	46.77%	3.402%
22	10.915	1685	1694	1697	rBV3	6209252	11311464	36.11%	2.627%
23	10.951	1697	1700	1705	rVB	7263620	9307210	29.71%	2.161%
24	11.006	1705	1709	1714	rVB3	2090286	3373553	10.77%	0.783%
25	11.061	1714	1718	1719	rBV2	2535812	3157172	10.08%	0.733%
26	11.085	1719	1722	1726	rVB2	4262227	5394513	17.22%	1.253%
27	11.140	1726	1731	1735	rVB	9930872	12925218	41.26%	3.001%
28	11.183	1735	1738	1741	rVB2	1999464	2342909	7.48%	0.544%
29	11.219	1741	1744	1746	rBV	1508392	1680066	5.36%	0.390%
30	11.280	1746	1754	1764	rVB3	9423521	16804141	53.65%	3.902%
31	11.360	1764	1767	1769	rBV2	782762	831613	2.65%	0.193%
32	11.396	1769	1773	1778	rBV4	3315991	6119158	19.54%	1.421%
33	11.451	1778	1782	1785	rBV2	2917008	4001897	12.78%	0.929%
34	11.488	1785	1788	1792	rBV	9293784	12060267	38.50%	2.801%

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35	11.542	1792	1797	1801	rVB4	6352886	10193356	32.54%	2.367%
36	11.585	1801	1804	1809	rVB4	1532448	2530645	8.08%	0.588%
37	11.634	1809	1812	1814	rBV	1374974	1607687	5.13%	0.373%
38	11.664	1814	1817	1818	rBV	1681471	1892226	6.04%	0.439%
39	11.689	1818	1821	1825	rVB5	6350644	8224756	26.26%	1.910%
40	11.744	1825	1830	1832	rBV2	6484424	8543963	27.28%	1.984%
41	11.780	1832	1836	1839	rVV	25357252	31324046	100.00%	7.274%
42	11.805	1839	1840	1843	rVV2	4531283	4801549	15.33%	1.115%
43	11.841	1843	1846	1851	rVB3	6776477	11020747	35.18%	2.559%
44	11.896	1851	1855	1858	rBV2	6480448	10248542	32.72%	2.380%
45	11.951	1860	1864	1868	rVB3	9845065	13934124	44.48%	3.236%
46	12.006	1868	1873	1876	rBV2	13107631	17653772	56.36%	4.100%
47	12.036	1876	1878	1883	rVB4	4391755	5872136	18.75%	1.364%
48	12.097	1883	1888	1891	rBV3	6558513	9174558	29.29%	2.131%
49	12.134	1891	1894	1897	rVB3	3769824	4495137	14.35%	1.044%
50	12.183	1897	1902	1903	rBV4	3027705	4732861	15.11%	1.099%
51	12.305	1918	1922	1927	rBV5	5150666	8531795	27.24%	1.981%
52	12.372	1927	1933	1940	rVV6	10242446	21308366	68.03%	4.948%
53	12.481	1940	1951	1955	rVV3	5641279	15662205	50.00%	3.637%
54	12.530	1955	1959	1964	rVB4	6416655	12000651	38.31%	2.787%
55	12.615	1967	1973	1975	rBV4	3989262	7827081	24.99%	1.818%
56	12.640	1975	1977	1980	rVV3	4119627	5836537	18.63%	1.355%
57	12.670	1980	1982	1990	rVB	6480699	9945243	31.75%	2.309%
58	12.743	1990	1994	1998	rBV3	3583512	6365069	20.32%	1.478%
59	12.823	2004	2007	2012	rBV4	1087812	2223155	7.10%	0.516%
60	12.878	2012	2016	2022	rVB5	6043780	10096773	32.23%	2.345%
61	12.945	2022	2027	2031	rBV3	6621754	11212188	35.79%	2.604%
62	12.981	2031	2033	2037	rVB2	4592588	4705681	15.02%	1.093%
63	13.024	2037	2040	2041	rBV2	913455	1070712	3.42%	0.249%
64	13.048	2041	2044	2047	rVV	3399717	4109918	13.12%	0.954%
65	13.085	2047	2050	2057	rVB3	2078658	3976466	12.69%	0.923%
66	13.152	2057	2061	2066	rBV3	1729148	2809761	8.97%	0.652%
67	13.201	2066	2069	2076	rVB3	1292430	1713051	5.47%	0.398%
68	13.310	2083	2087	2089	rBV3	1011509	1442220	4.60%	0.335%
69	13.347	2089	2093	2100	rVB2	5835153	9132689	29.16%	2.121%
70	13.426	2103	2106	2110	rVV2	951047	1527412	4.88%	0.355%
71	13.475	2111	2114	2125	rVB6	1398471	3213941	10.26%	0.746%

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72	13.566	2125	2129	2132	rBV3	535814	841422	2.69%	0.195%
73	13.597	2132	2134	2137	rVB	382890	443204	1.41%	0.103%
74	13.640	2137	2141	2146	rBV4	1164284	1783495	5.69%	0.414%
75	13.695	2146	2150	2152	rVV4	375962	677974	2.16%	0.157%
76	13.725	2152	2155	2160	rVB2	727361	1139846	3.64%	0.265%
77	13.804	2163	2168	2173	rVB2	418710	723370	2.31%	0.168%
78	13.853	2173	2176	2180	rVB2	386027	488814	1.56%	0.114%
79	13.902	2181	2184	2190	rVB3	230705	405961	1.30%	0.094%
80	13.987	2190	2198	2202	rVB4	330702	709703	2.27%	0.165%
81	14.274	2241	2245	2253	rVB3	196172	353053	1.13%	0.082%

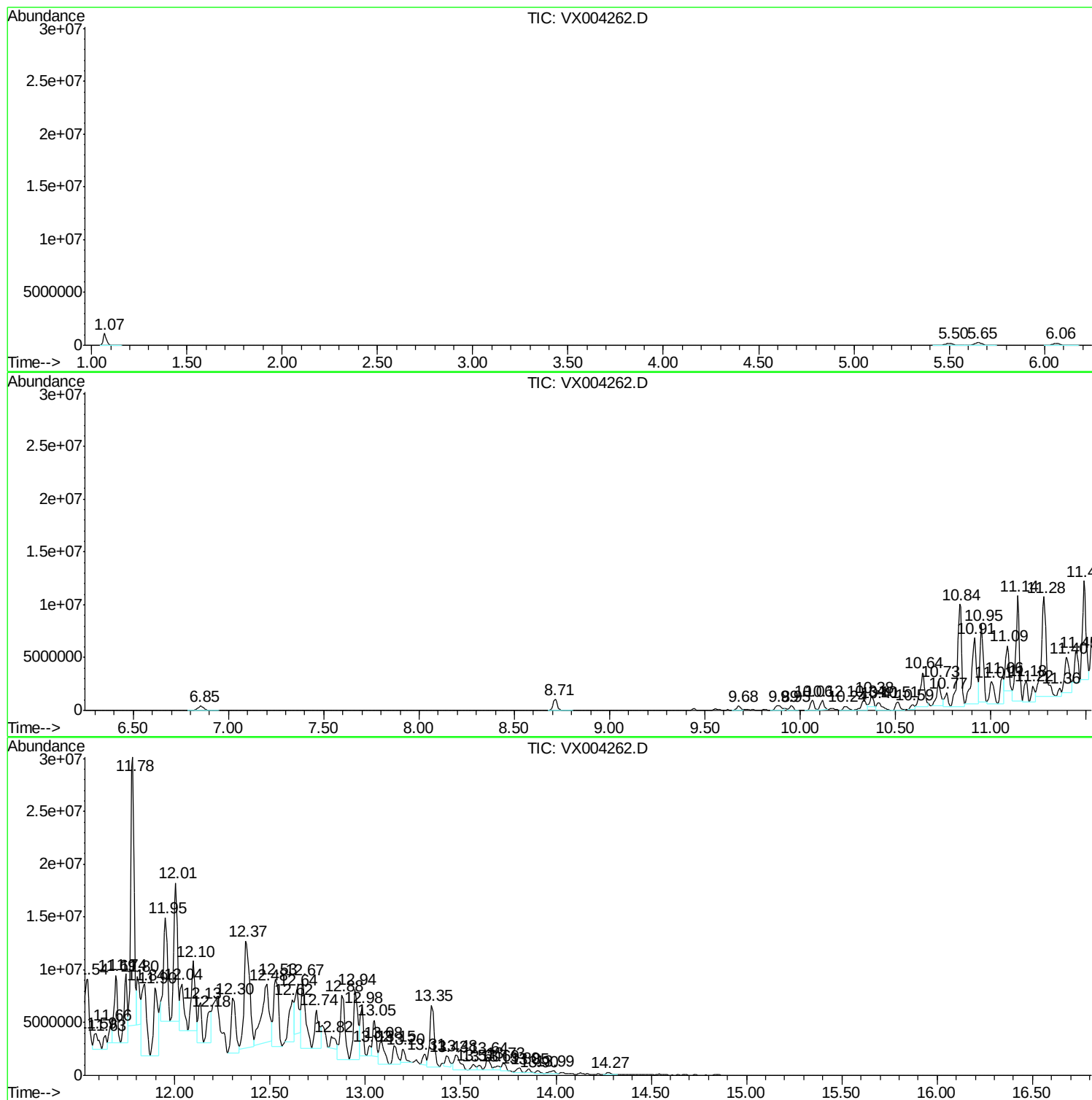
Sum of corrected areas: 430626139

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



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Peak Number 1 Octane, 2,5-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.		
10.73	146.29 ug/l	3699700	Chlorobenzene-d5	10.12		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2,5-dimethyl-	142	C10H22	015869-89-3	90	
2	Nonane, 4-methyl-	142	C10H22	017301-94-9	74	
3	Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	64	
4	Decane, 6-ethyl-2-methyl-	184	C13H28	062108-21-8	53	
5	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	52	

Peak Number 2 Octane, 2,6-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.84	579.27 ug/l	14649700	Chlorobenzene-d5	10.12	
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual	
1	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	93
2	Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	87
3	Nonane, 3-methyl-	142	C10H22	005911-04-6	87
4	Undecane, 4,5-dimethyl-	184	C13H28	017312-79-7	59
5	Sulfurous acid, di(2-ethylhexyl)...	306	C16H34O3S	1000309-19-1	53

Peak Number 3 Ethanone, 1-cyclohexyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.		
10.91	447.27 ug/l	11311500	Chlorobenzene-d5	10.12		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanone, 1-cyclohexyl-	126	C8H14O	000823-76-7	52	
2	Cyclohexane, propyl-	126	C9H18	001678-92-8	49	
3	Cyclohexane, (1-methylethyl)-	126	C9H18	000696-29-7	46	
4	Cyclohexane, methyl-	98	C7H14	000108-87-2	35	
5	4-Nonene	126	C9H18	002198-23-4	20	

Peak Number 4 Heptane, 4-propyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
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10.95	368.02 ug/l	9307210	Chlorobenzene-d5	10.12		
Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptane, 4-propyl-	142	C10H22	003178-29-8	64
2		Heptane, 4-(1-methylethyl)-	142	C10H22	052896-87-4	64
3		Undecane, 6-methyl-	170	C12H26	017302-33-9	64
4		Heptane, 3-ethyl-2-methyl-	142	C10H22	014676-29-0	58
5		Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	53

 Peak Number 5 Heptane, 3-ethyl-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.09	213.31 ug/l	5394510	Chlorobenzene-d5	10.12	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane, 3-ethyl-2-methyl-	142	C10H22	014676-29-0	59
2	1-Octanol, 2-butyl-	186	C12H26O	003913-02-8	53
3	Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	50
4	Undecane, 2,5-dimethyl-	184	C13H28	017301-22-3	50
5	Octane, 4-ethyl-	142	C10H22	015869-86-0	50

 Peak Number 6 2-Octene, 2,6-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.28	91.58 ug/l	16804100	1,4-Dichlorobenzene-d4	12.09	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Octene, 2,6-dimethyl-	140	C10H20	004057-42-5	70
2	4-Octene, 2,6-dimethyl-, [S-(E)]-	140	C10H20	062960-76-3	68
3	4-Octene, 2,6-dimethyl-, [S-(Z)]-	140	C10H20	062960-77-4	64
4	Cyclohexane, 1,1,4,4-tetramethyl-	140	C10H20	002223-52-1	53
5	Cyclohexane, 1,1,2,3-tetramethyl-	140	C10H20	006783-92-2	53

 Peak Number 7 Decane, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.		
11.78	170.71 ug/l	31324000	1,4-Dichlorobenzene-d4	12.09		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual

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1	Decane, 4-methyl-	156	C11H24	002847-72-5	90
2	Octane, 3,3-dimethyl-	142	C10H22	004110-44-5	72
3	Heptane, 5-ethyl-2-methyl-	142	C10H22	013475-78-0	64
4	Heptane, 2,5,5-trimethyl-	142	C10H22	001189-99-7	59
5	Bis(2-ethylhexyl) methylenesuccin...	354	C21H38O4	002287-83-4	59

Peak Number 8 Cyclohexane, butyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.01	96.21 ug/l	17653800	1,4-Dichlorobenzene-d4	12.09

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, butyl-	140	C10H20	001678-93-9	81
2			Cyclohexane, pentyl-	154	C11H22	004292-92-6	76
3			Cyclohexane, (2-methylpropyl)-	140	C10H20	001678-98-4	72
4			Cyclohexane, octyl-	196	C14H28	001795-15-9	72
5			Cyclohexane, decyl-	224	C16H32	001795-16-0	64

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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Octane, 2,5-dimet...	10.73	146.3	ug/l	3699700	3	10.12	1264500	50.0
Octane, 2,6-dimet...	10.84	579.3	ug/l	14649700	3	10.12	1264500	50.0
Ethanone, 1-cyclo...	10.91	447.3	ug/l	11311500	3	10.12	1264500	50.0
Heptane, 4-propyl-	10.95	368.0	ug/l	9307210	3	10.12	1264500	50.0
Heptane, 3-ethyl-...	11.09	213.3	ug/l	5394510	3	10.12	1264500	50.0
2-Octene, 2,6-dim...	11.28	91.6	ug/l	16804100	4	12.09	9174560	50.0
Decane, 4-methyl-	11.78	170.7	ug/l	31324000	4	12.09	9174560	50.0
Cyclohexane, butyl-	12.01	96.2	ug/l	17653800	4	12.09	9174560	50.0