

Data Path : W:\HPCHEM1\MSVOA X\DATA\X053118\
 Data File : VX002213.D
 Acq On : 01 Jun 2018 12:01
 Operator : JC/MD
 Sample : VSTDCCC050
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 45 Sample Multiplier: 1

Instrument :
 MSVOA_X
 LabSampleId :
 VSTDCCC050

Integration Parameters: RTEINT.P

Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : W:\HPCHEM1\MSVOA_X\METHOD\82X052418W.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	1.075	76	80	93	rBV	1026100	1296189	37.08%	1.236%
2	1.197	97	100	108	rVB	197068	202119	5.78%	0.193%
3	1.325	118	121	131	rVB	215448	232522	6.65%	0.222%
4	1.410	131	135	144	rBV	227455	266509	7.62%	0.254%
5	1.636	169	172	181	rVB	248737	268641	7.68%	0.256%
6	1.721	181	186	199	rVB	153038	218652	6.25%	0.209%
7	1.928	214	220	233	rBV	399662	593828	16.99%	0.566%
8	2.191	257	263	270	rBV	300567	433124	12.39%	0.413%
9	2.258	270	274	277	rVV	25717	41078	1.17%	0.039%
10	2.300	277	281	287	rVV	92072	143225	4.10%	0.137%
11	2.380	287	294	301	rVV2	706309	1372264	39.25%	1.309%
12	2.453	301	306	311	rVV	419673	699357	20.00%	0.667%
13	2.514	311	316	321	rVV	179132	332319	9.51%	0.317%
14	2.569	321	325	341	rVB	235812	426270	12.19%	0.407%
15	2.733	343	352	356	rBV	418382	777089	22.23%	0.741%
16	2.782	356	360	366	rVV	186356	330048	9.44%	0.315%
17	2.861	366	373	387	rVB	328890	655080	18.74%	0.625%
18	3.081	401	409	415	rBV	149382	327063	9.36%	0.312%
19	3.160	415	422	427	rVV2	800723	1840792	52.65%	1.756%
20	3.209	427	430	445	rVB	485185	1007551	28.82%	0.961%
21	3.702	501	511	522	rVB	251388	610664	17.47%	0.582%
22	3.831	522	532	537	rBV	1102191	2659784	76.08%	2.537%
23	4.599	641	658	668	rBV2	461430	1455497	41.63%	1.388%
24	4.715	668	677	684	rBV	317519	869403	24.87%	0.829%
25	4.800	684	691	697	rBV	184800	435406	12.45%	0.415%
26	4.879	697	704	718	rVB2	177124	659956	18.88%	0.629%
27	5.032	718	729	732	rBV	198452	579060	16.56%	0.552%
28	5.172	743	752	758	rBV	395232	1283872	36.72%	1.224%
29	5.507	791	807	813	rBV2	415153	1308263	37.42%	1.248%
30	5.580	813	819	827	rVV	341397	1009695	28.88%	0.963%
31	5.672	827	834	838	rVV	213774	607362	17.37%	0.579%
32	5.727	838	843	848	rVV	300084	854524	24.44%	0.815%
33	5.800	848	855	870	rVB2	484163	1495577	42.78%	1.426%
34	6.074	889	900	905	rBV	211593	534927	15.30%	0.510%

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35	6.147	905	912	918	rVV	507347	1370872	39.21%	1.307%
36	6.202	918	921	929	rVV	219465	477935	13.67%	0.456%
37	6.281	930	934	946	rVB2	18536	47717	1.36%	0.046%
38	6.470	954	965	984	rVB	292676	719175	20.57%	0.686%
39	6.867	1019	1030	1043	rBV	304301	723189	20.69%	0.690%
40	7.220	1078	1088	1100	rBV	433161	924609	26.45%	0.882%
41	7.464	1119	1128	1133	rBV	543571	1188139	33.98%	1.133%
42	7.519	1133	1137	1150	rVB	402267	816922	23.37%	0.779%
43	7.665	1153	1161	1170	rBV	282274	546223	15.62%	0.521%
44	7.781	1170	1180	1192	rVV2	430693	925962	26.49%	0.883%
45	7.897	1192	1199	1215	rVB2	554688	1187057	33.95%	1.132%
46	8.196	1241	1248	1261	rBV	98939	184130	5.27%	0.176%
47	8.318	1261	1268	1281	rVV	1498954	2334165	66.77%	2.226%
48	8.439	1281	1288	1295	rVV	511065	808216	23.12%	0.771%
49	8.513	1295	1300	1306	rVB2	26031	43644	1.25%	0.042%
50	8.659	1316	1324	1329	rBV	2061891	3279247	93.80%	3.127%
51	8.720	1329	1334	1340	rVV	1001861	1613685	46.16%	1.539%
52	8.787	1340	1345	1371	rVB	1039042	1664531	47.61%	1.588%
53	9.049	1381	1388	1393	rBV	530925	770282	22.03%	0.735%
54	9.183	1404	1410	1413	rBV	607281	858574	24.56%	0.819%
55	9.220	1413	1416	1429	rVB	625186	877037	25.09%	0.836%
56	9.342	1429	1436	1439	rBV	941283	1433799	41.01%	1.367%
57	9.378	1439	1442	1448	rVB	568046	779386	22.29%	0.743%
58	9.500	1457	1462	1471	rBV	1794534	2457369	70.29%	2.344%
59	9.586	1471	1476	1481	rVV	379079	567711	16.24%	0.541%
60	9.647	1481	1486	1489	rVV	653412	875473	25.04%	0.835%
61	9.677	1489	1491	1498	rVB	319274	386385	11.05%	0.369%
62	10.116	1557	1563	1565	rBV	655138	946138	27.06%	0.902%
63	10.140	1565	1567	1575	rVV	1013622	1326676	37.95%	1.265%
64	10.226	1575	1581	1583	rVV	754856	1028622	29.42%	0.981%
65	10.256	1583	1586	1597	rVV	1346233	1746171	49.95%	1.665%
66	10.360	1598	1603	1626	rVB	2434482	3496088	100.00%	3.334%
67	10.707	1653	1660	1670	rBV2	1920152	3331506	95.29%	3.177%
68	10.860	1679	1685	1689	rBV	352135	475185	13.59%	0.453%
69	10.902	1689	1692	1705	rVV	911277	1055283	30.18%	1.006%
70	11.024	1706	1712	1717	rVV	1480181	1919141	54.89%	1.830%
71	11.079	1717	1721	1726	rVV	477438	589669	16.87%	0.562%

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72	11.140	1726	1731	1745	rVV	938961	1214795	34.75%	1.159%
73	11.262	1745	1751	1755	rVV2	1112762	2031061	58.10%	1.937%
74	11.299	1755	1757	1764	rVV2	675343	1367583	39.12%	1.304%
75	11.366	1764	1768	1773	rVV	1562338	1882035	53.83%	1.795%
76	11.427	1773	1778	1784	rVV	1278447	1586441	45.38%	1.513%
77	11.512	1787	1792	1804	rVB2	2793150	3483867	99.65%	3.323%
78	11.774	1829	1835	1839	rBV2	1961470	2880520	82.39%	2.747%
79	11.811	1839	1841	1856	rVB	1655703	1772902	50.71%	1.691%
80	11.951	1858	1864	1870	rBV	1537521	1862997	53.29%	1.777%
81	12.030	1871	1877	1880	rBV	1178288	1472651	42.12%	1.405%
82	12.073	1880	1884	1887	rBV3	1760570	2918432	83.48%	2.783%
83	12.396	1931	1937	1947	rVB	2638657	3260331	93.26%	3.109%
84	12.603	1963	1971	1977	rBV	850121	1117335	31.96%	1.066%
85	12.823	2002	2007	2012	rBV2	81599	110873	3.17%	0.106%
86	13.006	2026	2037	2045	rBV2	323261	453502	12.97%	0.433%
87	13.164	2059	2063	2070	rVB2	28622	37244	1.07%	0.036%
88	13.347	2088	2093	2103	rVB	1699470	1966618	56.25%	1.876%
89	13.652	2136	2143	2151	rVB	1123215	1390138	39.76%	1.326%
90	13.786	2159	2165	2169	rBV	975577	1186150	33.93%	1.131%
91	13.841	2169	2174	2180	rVB	1349049	1672680	47.84%	1.595%
92	14.024	2198	2204	2210	rBV	1160416	1434554	41.03%	1.368%
93	14.188	2226	2231	2237	rBV	62150	87240	2.50%	0.083%
94	15.469	2435	2441	2447	rVB	36143	58746	1.68%	0.056%

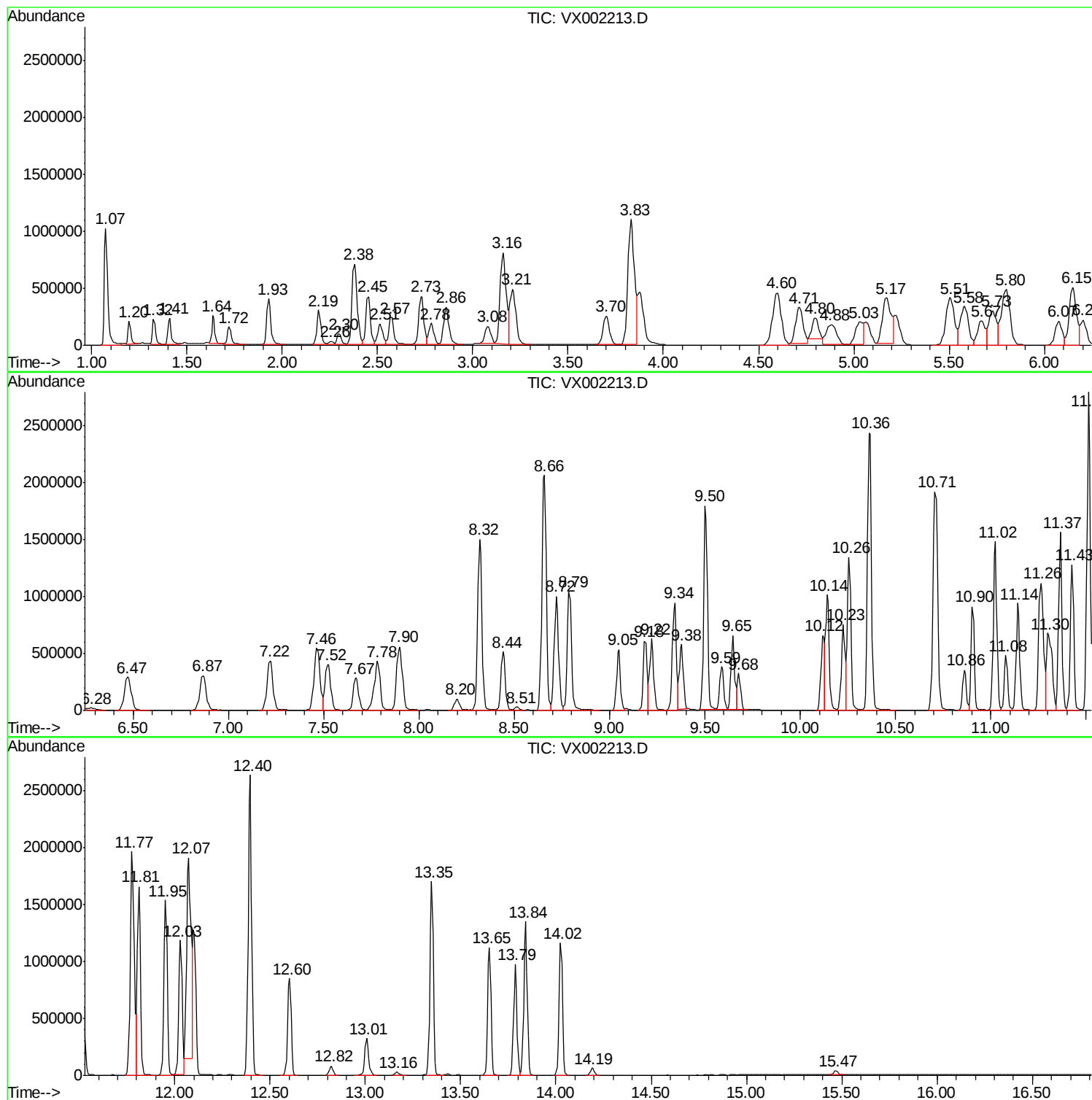
Sum of corrected areas: 104852318

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



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 Peak Number 1 Propanenitrile Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.80	35.84 ug/l	435406	Pentafluorobenzene	5.67

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Propanenitrile	55	C3H5N	000107-12-0	64
2		Propargylamine	55	C3H5N	002450-71-7	9
3		2-Butyne	54	C4H6	000503-17-3	9
4		1,2-Butadiene	54	C4H6	000590-19-2	5
5		1-Butyne	54	C4H6	000107-00-6	4

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.73	70.35 ug/l	854524	Pentafluorobenzene	5.67

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butane, 1-chloro-	92	C4H9Cl	000109-69-3	90
2		Cyclobutanecarbonitrile, 3,3-dim...	109	C7H11N	053783-86-1	45
3		3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	38
4		Oxetane, 3,3-dimethyl-	86	C5H10O	006921-35-3	36
5		Cyclobutane, ethyl-	84	C6H12	004806-61-5	12

 Peak Number 3 Propane, 1-nitro- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.20	12.73 ug/l	184130	1,4-Difluorobenzene	6.87

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Propane, 1-nitro-	89	C3H7NO2	000108-03-2	50
2		Propane, 2-nitro-	89	C3H7NO2	000079-46-9	28
3		Propene	42	C3H6	000115-07-1	9
4		Isobutyl nitrite	103	C4H9NO2	000542-56-3	9
5		Cyclopropanecarboxaldehyde	70	C4H6O	001489-69-6	9

 Peak Number 4 Benzene, 1,2,3,4-tetramethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
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13.35	33.69 ug/l	1966620	1,4-Dichlorobenzene-d4		12.09	
Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual

1		Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	97
2		Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	97
3		o-Cymene	134	C10H14	000527-84-4	95
4		Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	94
5		Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	94

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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propanenitrile	4.80	35.8	ug/l	435406	1	5.67	607362	50.0
Butane, 1-chloro-	5.73	70.3	ug/l	854524	1	5.67	607362	50.0
Propane, 1-nitro-	8.20	12.7	ug/l	184130	2	6.87	723189	50.0
Benzene, 1,2,3,4-...	13.35	33.7	ug/l	1966620	4	12.09	2918430	50.0