

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX061318\
 Data File : VX002543.D
 Acq On : 14 Jun 2018 07:34
 Operator : JC/MD
 Sample : J3413-09
 Misc : 7.27g/5mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 46 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 P-9R

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 : 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	92	rBV	972300	1243748	5.46%	0.401%
2	5.507	787	807	814	rBV2	170638	576474	2.53%	0.186%
3	5.659	826	832	856	rVB2	294502	1233804	5.41%	0.397%
4	6.336	934	943	953	rVB	270102	817952	3.59%	0.263%
5	6.860	1020	1029	1037	rBV	397954	1009020	4.43%	0.325%
6	7.458	1115	1127	1137	rBV2	278404	717310	3.15%	0.231%
7	8.055	1214	1225	1237	rVB	367064	862194	3.78%	0.278%
8	8.177	1237	1245	1253	rBV	473859	1030309	4.52%	0.332%
9	8.500	1293	1298	1307	rBV	363470	666464	2.92%	0.215%
10	8.677	1319	1327	1330	rBV3	412281	947077	4.15%	0.305%
11	8.720	1330	1334	1341	rVB	978900	1639577	7.19%	0.528%
12	9.561	1467	1472	1478	rBV3	342878	727908	3.19%	0.234%
13	9.963	1534	1538	1543	rVB	798149	1126604	4.94%	0.363%
14	10.067	1548	1555	1559	rBV	768689	1062902	4.66%	0.342%
15	10.116	1559	1563	1568	rBV	856116	1225248	5.38%	0.395%
16	10.256	1580	1586	1591	rVB	994611	1377875	6.04%	0.444%
17	10.366	1591	1604	1609	rBV2	1158321	2346193	10.29%	0.756%
18	10.414	1609	1612	1623	rVB	997898	1519277	6.67%	0.489%
19	10.646	1643	1650	1653	rBV3	565865	900970	3.95%	0.290%
20	10.835	1673	1681	1685	rBV2	934890	1490654	6.54%	0.480%
21	10.914	1685	1694	1698	rBV3	898821	1574355	6.91%	0.507%
22	11.140	1726	1731	1742	rVB5	1682803	3762982	16.51%	1.212%
23	11.250	1742	1749	1751	rBV	837297	1233374	5.41%	0.397%
24	11.280	1751	1754	1758	rVB4	625565	796653	3.49%	0.257%
25	11.365	1764	1768	1771	rBV	847471	1053468	4.62%	0.339%
26	11.445	1776	1781	1782	rVV	1525135	2115322	9.28%	0.681%
27	11.512	1786	1792	1794	rVV2	2790001	4444566	19.50%	1.431%
28	11.536	1794	1796	1801	rVB2	2988028	3182025	13.96%	1.025%
29	11.676	1814	1819	1826	rVB	1800454	2867521	12.58%	0.924%
30	11.774	1832	1835	1837	rBV	1188265	1213863	5.33%	0.391%
31	11.810	1837	1841	1851	rVB	9416011	12777955	56.06%	4.115%
32	11.951	1857	1864	1868	rBV3	935887	1515101	6.65%	0.488%
33	12.006	1868	1873	1875	rBV	1402605	1856923	8.15%	0.598%
34	12.030	1875	1877	1881	rVB2	934557	1061665	4.66%	0.342%

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35	12.085	1881	1886	1891	rBV3	1491346	2607551	11.44%	0.840%
36	12.152	1891	1897	1902	rVB3	2594951	4188987	18.38%	1.349%
37	12.231	1905	1910	1917	rVB3	1076007	2097037	9.20%	0.675%
38	12.304	1917	1922	1924	rBV2	2515053	3382953	14.84%	1.090%
39	12.329	1924	1926	1929	rVB	2017500	2041876	8.96%	0.658%
40	12.377	1929	1934	1940	rVB4	5024160	7813537	34.28%	2.516%
41	12.481	1940	1951	1955	rBV	3154023	4905477	21.52%	1.580%
42	12.524	1955	1958	1964	rVB2	2248812	3283021	14.40%	1.057%
43	12.591	1964	1969	1971	rBV	2252000	3005485	13.18%	0.968%
44	12.615	1971	1973	1979	rVB	2400188	2600965	11.41%	0.838%
45	12.676	1979	1983	1986	rVB	2822099	3143842	13.79%	1.013%
46	12.762	1991	1997	1999	rBV2	1625505	2821756	12.38%	0.909%
47	12.883	2010	2017	2019	rVV3	1568372	2867340	12.58%	0.923%
48	12.908	2019	2021	2024	rVB2	883540	919460	4.03%	0.296%
49	12.951	2024	2028	2030	rBV2	1763119	2596103	11.39%	0.836%
50	12.981	2030	2033	2037	rVV	2208792	3167482	13.90%	1.020%
51	13.024	2037	2040	2047	rVB2	3402829	5866505	25.74%	1.889%
52	13.103	2047	2053	2056	rBV4	1511925	3002921	13.17%	0.967%
53	13.225	2066	2073	2078	rBV4	2152819	3952339	17.34%	1.273%
54	13.274	2078	2081	2084	rVB	1385249	1405193	6.16%	0.453%
55	13.316	2084	2088	2091	rBV3	1568408	2748579	12.06%	0.885%
56	13.353	2091	2094	2099	rVV2	6025454	8684429	38.10%	2.797%
57	13.438	2104	2108	2112	rVV2	1020205	1600446	7.02%	0.515%
58	13.487	2112	2116	2124	rVB4	3501633	6805686	29.86%	2.192%
59	13.566	2125	2129	2132	rBV2	1367381	2003305	8.79%	0.645%
60	13.609	2132	2136	2138	rBV	1338464	1673589	7.34%	0.539%
61	13.646	2138	2142	2147	rBV3	2050382	3426084	15.03%	1.103%
62	13.731	2153	2156	2160	rVB2	1632481	2342359	10.28%	0.754%
63	13.841	2170	2174	2180	rVB	2632386	4084964	17.92%	1.316%
64	13.914	2180	2186	2191	rVB3	2707993	5653054	24.80%	1.821%
65	13.993	2191	2199	2203	rBV4	3028829	5848083	25.66%	1.883%
66	14.036	2203	2206	2209	rBV2	794548	1017080	4.46%	0.328%
67	14.072	2209	2212	2214	rVV	655776	958715	4.21%	0.309%
68	14.139	2218	2223	2226	rBV3	2705274	3756389	16.48%	1.210%
69	14.170	2226	2228	2231	rVB2	650164	609518	2.67%	0.196%
70	14.225	2235	2237	2241	rVV	776155	855792	3.75%	0.276%
71	14.292	2242	2248	2254	rVB2	4988886	9730497	42.69%	3.134%

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72	14.383	2260	2263	2268	rBV3	1828617	2448457	10.74%	0.789%
73	14.438	2268	2272	2276	rVB	2681772	3018738	13.24%	0.972%
74	14.487	2276	2280	2285	rVB5	1221494	2342491	10.28%	0.754%
75	14.548	2285	2290	2298	rBV3	3435271	6500224	28.52%	2.093%
76	14.621	2298	2302	2304	rBV3	668772	1027059	4.51%	0.331%
77	14.706	2308	2316	2319	rBV2	13668355	22794792	100.00%	7.341%
78	14.737	2319	2321	2326	rVB3	2866359	3583467	15.72%	1.154%
79	14.792	2326	2330	2333	rBV3	1803118	2624621	11.51%	0.845%
80	14.847	2335	2339	2343	rVV	7416447	9434214	41.39%	3.038%
81	14.883	2343	2345	2348	rVV2	1159529	1443004	6.33%	0.465%
82	14.914	2348	2350	2354	rVB3	1805007	1981087	8.69%	0.638%
83	14.968	2356	2359	2366	rVV2	803530	1435073	6.30%	0.462%
84	15.121	2378	2384	2387	rBV3	902494	1683754	7.39%	0.542%
85	15.255	2401	2406	2409	rBV	2958777	4896285	21.48%	1.577%
86	15.322	2414	2417	2419	rBV3	573448	802147	3.52%	0.258%
87	15.456	2434	2439	2442	rBV	3635589	5508057	24.16%	1.774%
88	15.487	2442	2444	2449	rVV3	948575	1475838	6.47%	0.475%
89	15.560	2450	2456	2461	rVB	7505584	11398053	50.00%	3.671%
90	15.700	2473	2479	2482	rBV	7253280	11348067	49.78%	3.655%
91	15.737	2482	2485	2493	rVB	4807568	7413171	32.52%	2.388%
92	15.926	2509	2516	2531	rVB2	1922398	5785838	25.38%	1.863%
93	16.078	2537	2541	2546	rBV	1072182	1774656	7.79%	0.572%
94	16.182	2553	2558	2564	rBV	1002419	1713202	7.52%	0.552%
95	16.285	2572	2575	2583	rVB2	765197	1368622	6.00%	0.441%
96	16.365	2583	2588	2590	rBV	389799	722843	3.17%	0.233%
97	16.450	2597	2602	2610	rVB	1346997	2558283	11.22%	0.824%
98	16.663	2632	2637	2639	rBV3	420553	707926	3.11%	0.228%
99	16.700	2639	2643	2648	rVB	997824	1797087	7.88%	0.579%
100	16.767	2648	2654	2657	rBV	844241	1465726	6.43%	0.472%

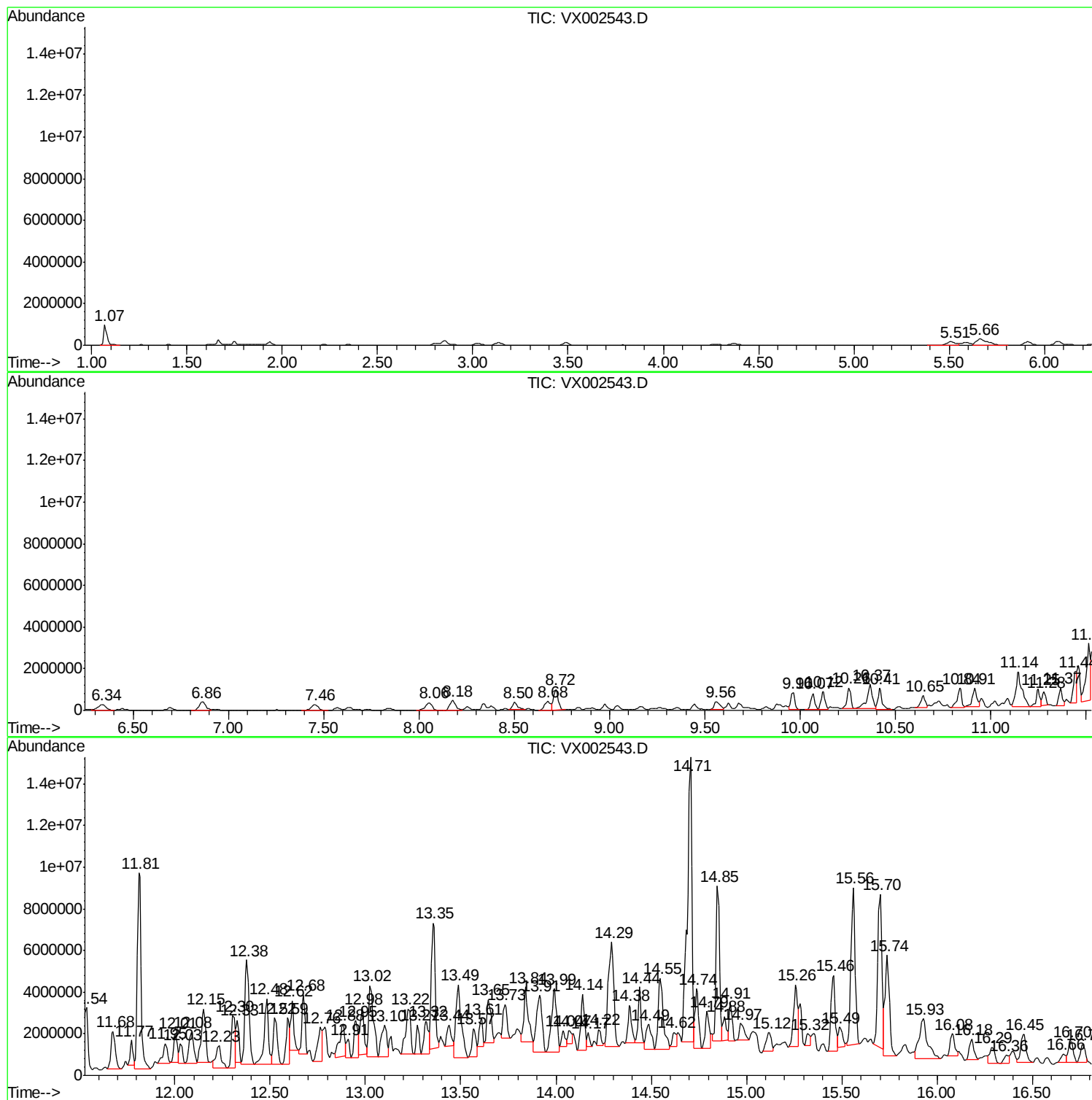
Sum of corrected areas: 310498514

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Quant Method : Z:\V0ASRV\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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Peak Number 1 Benzene, 1-ethyl-3,5-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.38	149.83 ug/l	7813540	1,4-Dichlorobenzene-d4	12.08
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzene, 1-ethyl-3,5-dimethyl-	134 C10H14	000934-74-7 95
2		Benzene, 1-methyl-3-(1-methyleth...	134 C10H14	000535-77-3 95
3		o-Cymene	134 C10H14	000527-84-4 94
4		Benzene, 1-ethyl-2,3-dimethyl-	134 C10H14	000933-98-2 94
5		Benzene, 1-ethyl-2,4-dimethyl-	134 C10H14	000874-41-9 93

Peak Number 2 1-Phenyl-1-butene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.35	166.53 ug/l	8684430	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 91
2		Benzene, 1-ethenyl-3-ethyl-	132 C10H12	007525-62-4 87
3		Benzene, (2-methylcyclopropyl)-	132 C10H12	1000327-39-0 86
4		1H-Indene, 2,3-dihydro-4-methyl-	132 C10H12	000824-22-6 86
5		1H-Indene, 2,3-dihydro-5-methyl-	132 C10H12	000874-35-1 86

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.49	130.50 ug/l	6805690	1,4-Dichlorobenzene-d4	12.08
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Naphthalene, 1,2,3,4-tetrahydro-	132 C10H12	000119-64-2 86
2		2H-Inden-2-one, 1,3-dihydro-	132 C9H8O	000615-13-4 43
3		Benzene, cyclobutyl-	132 C10H12	004392-30-7 38
4		Butanedioic acid, phenyl-	194 C10H10O4	000635-51-8 27
5		3(2H)-Furanone, dihydro-2,2-dime...	190 C12H14O2	063678-00-2 27

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
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14.29	186.58 ug/l	9730500	1,4-Dichlorobenzene-d4	12.08			
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	95
2			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	95
3			Benzene, 2-ethenyl-1,3,5-trimethyl-	146	C11H14	000769-25-5	86
4			Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	70
5			1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	70

 Peak Number 5 Naphthalene, 1-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.		
14.71	437.09 ug/l	22794800	1,4-Dichlorobenzene-d4	12.08		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2		Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3		Benzocycloheptatriene	142	C11H10	000264-09-5	91
4		1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
5		1-Ethanone, 1-[4-(1-naphthalenyl)...]	276	C19H16O2	1000338-30-5	47

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

R.T.	EstConc	Area	Relative to ISTD	R.T.		
15.56	218.56 ug/l	11398100	1,4-Dichlorobenzene-d4	12.08		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	97
2		Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	97
3		Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	96
4		Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	96
5		Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	96

 Peak Number 7 Naphthalene, 2,3-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.		
15.70	217.60 ug/l	11348100	1,4-Dichlorobenzene-d4	12.08		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual

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1	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	97
2	Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	97
3	Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	97
4	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	97
5	Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	97

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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Benzene, 1-ethyl-...	12.38	149.8	ug/l	7813540	4	12.08	2607550	50.0
1-Phenyl-1-butene	13.35	166.5	ug/l	8684430	4	12.08	2607550	50.0
Naphthalene, 1,2,...	13.49	130.5	ug/l	6805690	4	12.08	2607550	50.0
Naphthalene, 1,2,...	14.29	186.6	ug/l	9730500	4	12.08	2607550	50.0
Naphthalene, 1-me...	14.71	437.1	ug/l	22794800	4	12.08	2607550	50.0
Naphthalene, 2,6-...	15.56	218.6	ug/l	11398100	4	12.08	2607550	50.0
Naphthalene, 2,3-...	15.70	217.6	ug/l	11348100	4	12.08	2607550	50.0