

Data Path : Z:\VOASRV\HPCHEM1\MSVOA W\DATA\VW021119\
 Data File : VW008600.D
 Acq On : 11 Feb 2019 16:28
 Operator : SY/VA
 Sample : K1458-08
 Misc : 5.00G/5ML/MSVOA W/SOIL
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 SB-5

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_W\METHOD\82W012419S.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	2.117	34	35	39	rBV3	1175	1392	1.30%	0.185%
2	2.215	45	51	52	rBV5	11172	16633	15.58%	2.215%
3	2.843	153	154	159	rVB5	2105	2250	2.11%	0.300%
4	3.074	190	192	194	rBV4	1554	1333	1.25%	0.178%
5	3.099	194	196	200	rVB5	1858	2225	2.08%	0.296%
6	3.422	246	249	251	rBV4	1595	1283	1.20%	0.171%
7	3.477	257	258	261	rBV3	1180	1337	1.25%	0.178%
8	3.574	272	274	278	rVB5	1436	2026	1.90%	0.270%
9	3.897	324	327	329	rVB4	1390	1677	1.57%	0.223%
10	3.952	335	336	339	rBV3	1210	1203	1.13%	0.160%
11	4.044	350	351	355	rVB4	1689	1640	1.54%	0.218%
12	4.117	361	363	366	rBV3	1646	1305	1.22%	0.174%
13	4.336	396	399	400	rVB3	1575	1348	1.26%	0.180%
14	4.489	423	424	427	rVB3	2199	1911	1.79%	0.255%
15	4.525	427	430	433	rBV4	1435	1739	1.63%	0.232%
16	4.568	433	437	440	rVV5	1299	2320	2.17%	0.309%
17	4.604	440	443	445	rVV2	1529	1757	1.65%	0.234%
18	4.653	445	451	452	rVV6	1536	2578	2.41%	0.343%
19	4.702	456	459	461	rVB3	1950	1631	1.53%	0.217%
20	4.751	464	467	473	rVB8	1553	3086	2.89%	0.411%
21	4.903	488	492	493	rBV4	2153	3183	2.98%	0.424%
22	5.177	534	537	538	rBV3	1369	1395	1.31%	0.186%
23	5.440	578	580	583	rVB4	1672	1623	1.52%	0.216%
24	5.476	583	586	589	rBV5	1952	3595	3.37%	0.479%
25	5.610	606	608	611	rVB2	1650	1309	1.23%	0.174%
26	5.860	645	649	652	rBV4	1601	2383	2.23%	0.317%
27	5.903	652	656	658	rBV5	1488	2190	2.05%	0.292%
28	5.933	658	661	662	rBV3	2533	2538	2.38%	0.338%
29	6.305	721	722	725	rBV3	1687	1451	1.36%	0.193%
30	6.439	740	744	746	rBV3	1999	2937	2.75%	0.391%
31	6.500	752	754	758	rVB5	1336	1390	1.30%	0.185%
32	6.610	770	772	774	rVB2	1397	1221	1.14%	0.163%
33	6.830	806	808	810	rVB3	1744	1252	1.17%	0.167%
34	6.860	810	813	814	rBV2	2256	2092	1.96%	0.279%

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35	7.037	840	842	844	rBV3	2017	1530	1.43%	0.204%
36	7.086	847	850	851	rBV3	1365	1593	1.49%	0.212%
37	7.104	851	853	855	rBV3	1927	2027	1.90%	0.270%
38	7.201	866	869	871	rBV4	1347	1403	1.31%	0.187%
39	7.262	876	879	883	rVB5	1418	1752	1.64%	0.233%
40	7.305	883	886	888	rBV4	1465	1274	1.19%	0.170%
41	7.366	894	896	899	rBV4	1393	1294	1.21%	0.172%
42	7.409	902	903	907	rVB3	1306	1605	1.50%	0.214%
43	7.610	933	936	939	rBV5	1068	1692	1.58%	0.225%
44	7.781	962	964	968	rVB4	1361	1372	1.28%	0.183%
45	7.817	968	970	973	rVB4	1532	1622	1.52%	0.216%
46	7.890	973	982	986	rBV2	15657	41797	39.14%	5.566%
47	7.945	986	991	999	rVB2	28251	63081	59.07%	8.401%
48	8.104	1015	1017	1019	rVB3	1395	1386	1.30%	0.185%
49	8.134	1019	1022	1024	rBV3	1402	1525	1.43%	0.203%
50	8.165	1024	1027	1030	rVB5	1427	1899	1.78%	0.253%
51	8.244	1037	1040	1043	rVB5	1465	1300	1.22%	0.173%
52	8.305	1043	1050	1057	rBV2	16840	36230	33.93%	4.825%
53	8.573	1090	1094	1097	rBV5	1776	1682	1.58%	0.224%
54	8.665	1107	1109	1112	rBV4	1681	2410	2.26%	0.321%
55	8.695	1112	1114	1118	rVV4	2401	3261	3.05%	0.434%
56	8.750	1121	1123	1126	rVB4	1531	1554	1.46%	0.207%
57	8.835	1132	1137	1146	rVB	36651	75424	70.63%	10.045%
58	8.945	1153	1155	1161	rVB6	1203	1722	1.61%	0.229%
59	9.012	1165	1166	1171	rBV4	948	1342	1.26%	0.179%
60	9.055	1171	1173	1175	rBV3	1734	1339	1.25%	0.178%
61	9.536	1250	1252	1255	rBV3	1153	1417	1.33%	0.189%
62	9.646	1265	1270	1272	rBV4	1382	1912	1.79%	0.255%
63	9.738	1281	1285	1286	rBV2	1411	1449	1.36%	0.193%
64	9.908	1308	1313	1315	rBV6	1569	2397	2.24%	0.319%
65	10.000	1325	1328	1331	rVB4	1988	2391	2.24%	0.318%
66	10.049	1331	1336	1338	rBV6	1872	2645	2.48%	0.352%
67	10.079	1338	1341	1342	rBV3	1900	1818	1.70%	0.242%
68	10.097	1342	1344	1349	rVB5	2010	2773	2.60%	0.369%
69	10.323	1374	1381	1390	rVB	58591	106790	100.00%	14.222%
70	10.500	1408	1410	1413	rBV4	2215	2284	2.14%	0.304%
71	10.530	1413	1415	1416	rVB2	1909	1333	1.25%	0.178%

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72	10.567	1419	1421	1424	rVB4	1764	1652	1.55%	0.220%
73	10.603	1426	1427	1429	rBV2	1259	1212	1.13%	0.161%
74	10.658	1433	1436	1438	rBV4	2199	2579	2.42%	0.343%
75	10.701	1438	1443	1444	rBV4	2056	2778	2.60%	0.370%
76	10.896	1472	1475	1476	rBV3	1470	1431	1.34%	0.191%
77	10.933	1479	1481	1484	rVB4	1693	1431	1.34%	0.191%
78	10.975	1484	1488	1489	rBV2	1048	1380	1.29%	0.184%
79	11.061	1498	1502	1504	rBV5	1773	2209	2.07%	0.294%
80	11.560	1582	1584	1587	rVB4	2610	2198	2.06%	0.293%
81	11.628	1588	1595	1602	rVB	52966	92429	86.55%	12.310%
82	12.018	1657	1659	1662	rBV4	1628	1800	1.69%	0.240%
83	12.134	1674	1678	1683	rBV6	2087	3752	3.51%	0.500%
84	12.219	1690	1692	1695	rBV2	3081	3203	3.00%	0.427%
85	12.341	1708	1712	1714	rBV5	3581	3854	3.61%	0.513%
86	12.536	1741	1744	1745	rBV3	2443	2013	1.89%	0.268%
87	12.615	1751	1757	1766	rBV2	41617	77556	72.62%	10.329%
88	13.292	1864	1868	1869	rBV4	2760	2732	2.56%	0.364%
89	13.322	1871	1873	1874	rBV2	2745	2257	2.11%	0.301%
90	13.560	1906	1912	1920	rBV2	37479	65574	61.40%	8.733%
91	13.749	1941	1943	1945	rBV3	2865	2023	1.89%	0.269%
92	14.237	2021	2023	2026	rBV3	2125	1680	1.57%	0.224%
93	14.554	2073	2075	2076	rVB2	2835	1326	1.24%	0.177%
94	14.572	2076	2078	2079	rBV2	2404	1307	1.22%	0.174%
95	15.413	2214	2216	2217	rBV2	2646	2179	2.04%	0.290%
96	15.919	2297	2299	2301	rBV3	2458	1616	1.51%	0.215%
97	16.005	2311	2313	2318	rVB6	3150	3414	3.20%	0.455%
98	16.133	2333	2334	2336	rBV2	2449	1501	1.41%	0.200%
99	16.438	2382	2384	2385	rBV2	2685	1862	1.74%	0.248%
100	16.535	2398	2400	2403	rBV4	2870	2361	2.21%	0.314%

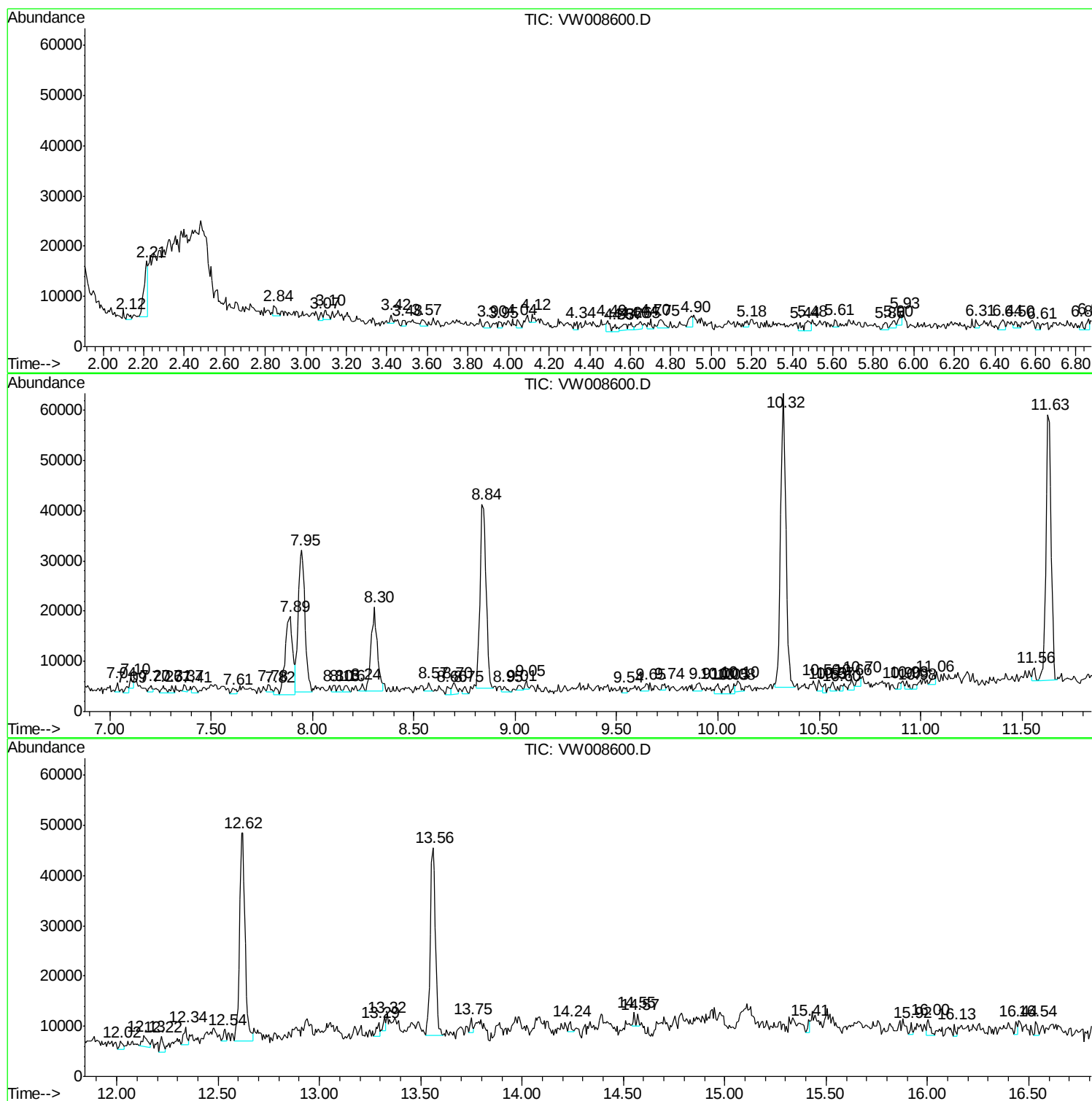
Sum of corrected areas: 750867

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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_W\METHOD\82W012419S.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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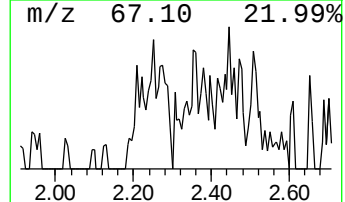
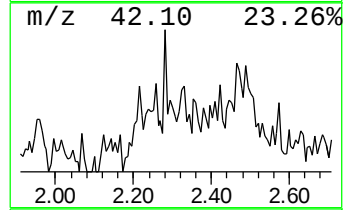
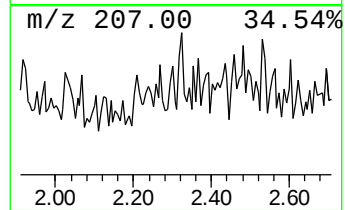
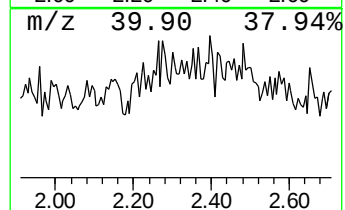
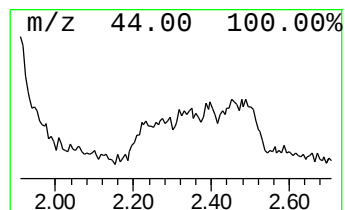
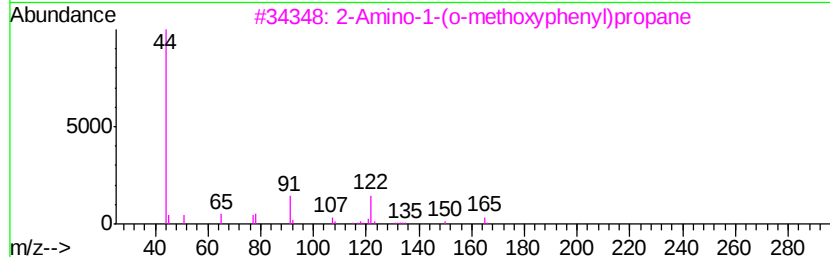
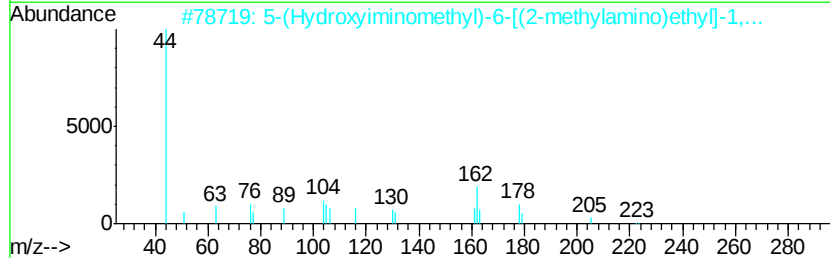
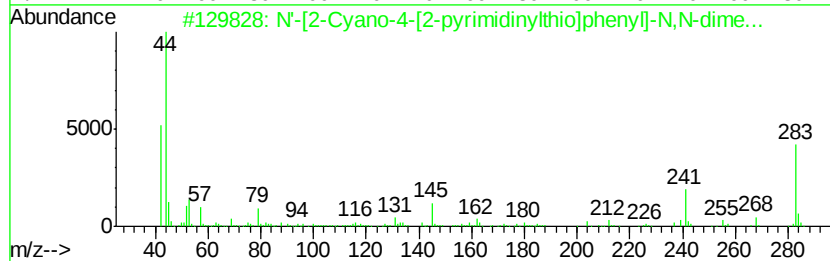
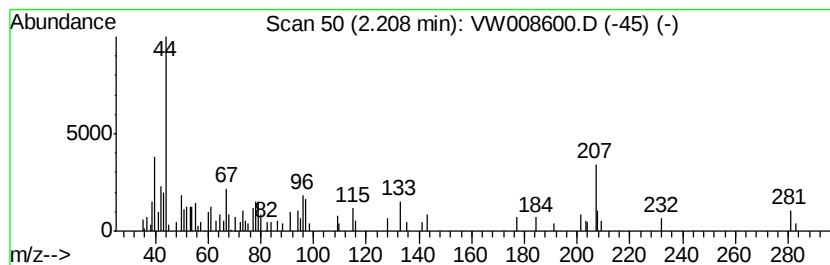
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_W\METHOD\82W012419S.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 N'-[2-Cyano-4-[2-pyrimidiny... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.21	13.18 ug/l	16633	Pentafluorobenzene	7.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	N'-[2-Cyano-4-[2-pyrimidinylthio]phenyl]-N,N-dimethyl-5-(hydroxymethyl)-6-[(2-methylamino)ethyl]-1,3,4-dihydro-2H-1,2,4-triazine-2-thione	283	C14H13N5S	074396-44-4	50
2		5-(Hydroxymethyl)-6-[(2-methylamino)ethyl]-1,3,4-dihydro-2H-1,2,4-triazine-2-thione	222	C11H14N2O3	007010-80-2	37
3		2-Amino-1-(o-methoxyphenyl)propane	165	C10H15NO	015402-84-3	37
4		Pyrido[3,4-d]imidazole, 1,6-dicarbonyl	211	C8H9N3O4	1000126-42-1	37
5		1-Pentanol, 4-amino-	103	C5H13NO	000927-55-9	33



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
N'-[2-Cyano-4-[2-...	2.21	13.2	ug/l	16633	1	7.95	63081	50.0