

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW082622\
 Data File : VW024405.D
 Acq On : 27 Aug 2022 16:57
 Operator : SY/VA
 Sample : N4363-09
 Misc : 4.39g/10mL/MSVOA_W/SOIL
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 DBVW4

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % 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_W\Method\SFAMWLM082622SMA.M
 Title : SFAM01.0

Signal : TIC: VW024405.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.343	67	72	83	rVB	130569	225077	17.84%	2.407%
2	2.873	154	159	168	rVB	84835	173762	13.77%	1.859%
3	3.666	287	289	290	rVB2	1445	781	0.06%	0.008%
4	3.708	294	296	297	rBV2	1468	1470	0.12%	0.016%
5	3.873	321	323	324	rBV2	1500	894	0.07%	0.010%
6	4.007	335	345	361	rBV	110943	340612	26.99%	3.643%
7	4.348	399	401	402	rBV2	1219	855	0.07%	0.009%
8	4.598	438	442	443	rBV3	1375	1439	0.11%	0.015%
9	4.702	457	459	460	rBV2	1053	757	0.06%	0.008%
10	4.751	465	467	468	rBV2	1372	1031	0.08%	0.011%
11	4.909	480	493	509	rBV4	19048	68918	5.46%	0.737%
12	5.050	514	516	518	rBV2	989	793	0.06%	0.008%
13	5.117	518	527	533	rBV7	4698	14906	1.18%	0.159%
14	5.385	568	571	572	rBV3	1063	1081	0.09%	0.012%
15	5.495	587	589	590	rBV2	1205	964	0.08%	0.010%
16	5.580	601	603	608	rVV6	950	1243	0.10%	0.013%
17	5.623	608	610	615	rVB5	1421	1739	0.14%	0.019%
18	5.720	624	626	628	rBV3	1229	1402	0.11%	0.015%
19	5.751	628	631	632	rVV3	1082	1244	0.10%	0.013%
20	5.787	635	637	640	rBV3	1400	1441	0.11%	0.015%
21	5.818	640	642	644	rBV3	1668	1349	0.11%	0.014%
22	6.043	677	679	681	rVB3	1385	1059	0.08%	0.011%
23	6.116	689	691	692	rVB2	2220	1099	0.09%	0.012%
24	6.135	692	694	695	rBV2	1249	801	0.06%	0.009%
25	6.159	695	698	699	rBV3	1086	823	0.07%	0.009%
26	6.500	752	754	755	rVB2	1406	888	0.07%	0.009%
27	6.592	764	769	770	rBV5	1179	1896	0.15%	0.020%
28	6.610	770	772	775	rBV4	749	782	0.06%	0.008%
29	6.653	775	779	780	rBV3	1166	1280	0.10%	0.014%
30	6.732	790	792	796	rBV5	1547	2011	0.16%	0.022%
31	6.805	801	804	807	rVB5	884	1081	0.09%	0.012%
32	6.897	816	819	821	rBV3	1722	2225	0.18%	0.024%
33	6.994	834	835	838	rBV3	1235	1175	0.09%	0.013%
34	7.031	838	841	842	rBV3	1698	1305	0.10%	0.014%
35	7.080	842	849	855	rBV	29973	81783	6.48%	0.875%
36	7.256	876	878	881	rBV4	1251	1232	0.10%	0.013%

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Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM082622SMA.M
 Title : SFAM01.0

37	7.482	913	915	919	rBV5	1237	1633	0.13%	0.017%
38	7.647	933	942	955	rVB	194916	468912	37.16%	5.015%
39	7.738	955	957	959	rVB3	1796	1114	0.09%	0.012%
40	8.025	1003	1004	1007	rVB3	1893	1065	0.08%	0.011%
41	8.055	1007	1009	1012	rVB4	1376	1329	0.11%	0.014%
42	8.177	1027	1029	1030	rBV2	1076	856	0.07%	0.009%
43	8.268	1036	1044	1062	rBV2	369570	1099082	87.10%	11.756%
44	8.841	1129	1138	1148	rBV	482012	970703	76.93%	10.383%
45	9.274	1200	1209	1218	rBV	246760	518537	41.09%	5.546%
46	9.451	1236	1238	1239	rBV2	898	847	0.07%	0.009%
47	9.975	1321	1324	1326	rBV4	1010	1163	0.09%	0.012%
48	10.036	1326	1334	1342	rVV	119805	229422	18.18%	2.454%
49	10.122	1343	1348	1356	rVB4	8666	16791	1.33%	0.180%
50	10.323	1374	1381	1389	rBV	546304	937927	74.33%	10.032%
51	10.579	1416	1423	1428	rBV	79460	139508	11.06%	1.492%
52	10.701	1439	1443	1450	rVB3	10519	17665	1.40%	0.189%
53	10.859	1463	1469	1474	rBV2	28436	48136	3.81%	0.515%
54	10.927	1474	1480	1487	rVV	112783	199018	15.77%	2.129%
55	11.061	1497	1502	1510	rBV3	33473	63271	5.01%	0.677%
56	11.274	1535	1537	1542	rBV6	1682	2260	0.18%	0.024%
57	11.372	1551	1553	1555	rBV3	991	791	0.06%	0.008%
58	11.530	1577	1579	1581	rBV3	1357	1226	0.10%	0.013%
59	11.628	1587	1595	1608	rBV	755473	1261853	100.00%	13.497%
60	11.786	1619	1621	1623	rBV3	1070	903	0.07%	0.010%
61	12.048	1662	1664	1666	rBV3	1318	995	0.08%	0.011%
62	12.280	1700	1702	1704	rBV3	1103	1164	0.09%	0.012%
63	12.414	1718	1724	1726	rVB7	1292	1931	0.15%	0.021%
64	12.432	1726	1727	1728	rBV	1385	672	0.05%	0.007%
65	12.457	1728	1731	1732	rBV2	1905	2432	0.19%	0.026%
66	12.597	1750	1754	1760	rVB2	12670	21632	1.71%	0.231%
67	12.688	1760	1769	1776	rBV	206681	341258	27.04%	3.650%
68	12.755	1776	1780	1782	rBV5	1065	1301	0.10%	0.014%
69	12.835	1791	1793	1794	rBV2	882	898	0.07%	0.010%
70	12.926	1804	1808	1815	rVB8	5603	9354	0.74%	0.100%
71	13.146	1842	1844	1846	rBV3	905	783	0.06%	0.008%
72	13.365	1875	1880	1881	rBV4	986	1682	0.13%	0.018%
73	13.389	1882	1884	1891	rVB8	4133	7432	0.59%	0.079%
74	13.469	1891	1897	1898	rBV6	1436	2211	0.18%	0.024%
75	13.554	1905	1911	1923	rVB	746317	1186862	94.06%	12.695%
76	13.853	1953	1960	1967	rBV	466314	770845	61.09%	8.245%

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 Title : SFAM01.0

77	14.066	1992	1995	1999	rVB3	4707	5715	0.45%	0.061%
78	14.164	2009	2011	2012	rBV2	1189	815	0.06%	0.009%
79	14.188	2012	2015	2017	rVV4	1496	1643	0.13%	0.018%
80	14.231	2020	2022	2024	rBV3	1473	1451	0.11%	0.016%
81	14.322	2032	2037	2043	rVB9	9478	15761	1.25%	0.169%
82	14.517	2066	2069	2071	rBV3	1512	1816	0.14%	0.019%
83	14.621	2081	2086	2087	rBV5	2107	3534	0.28%	0.038%
84	14.712	2098	2101	2106	rVV6	3543	3884	0.31%	0.042%
85	14.956	2139	2141	2145	rVB5	1528	1584	0.13%	0.017%
86	15.005	2147	2149	2151	rBV3	811	766	0.06%	0.008%
87	15.127	2163	2169	2173	rVB8	2822	4237	0.34%	0.045%
88	15.170	2173	2176	2182	rBV8	3100	5204	0.41%	0.056%
89	15.359	2205	2207	2210	rBV4	2126	1937	0.15%	0.021%
90	15.426	2215	2218	2224	rVB5	4176	7271	0.58%	0.078%
91	15.548	2234	2238	2243	rVB8	3018	6706	0.53%	0.072%
92	15.670	2255	2258	2259	rBV3	1176	1111	0.09%	0.012%
93	15.834	2282	2285	2287	rBV4	1579	1677	0.13%	0.018%
94	15.883	2291	2293	2294	rBV2	1396	865	0.07%	0.009%
95	15.938	2300	2302	2304	rBV3	1356	1264	0.10%	0.014%
96	15.999	2311	2312	2314	rBV2	1838	1400	0.11%	0.015%
97	16.133	2332	2334	2335	rVB2	1676	800	0.06%	0.009%
98	16.163	2338	2339	2341	rBV2	1441	905	0.07%	0.010%
99	16.200	2341	2345	2346	rBV4	1373	1593	0.13%	0.017%
100	16.285	2357	2359	2362	rBV4	880	709	0.06%	0.008%

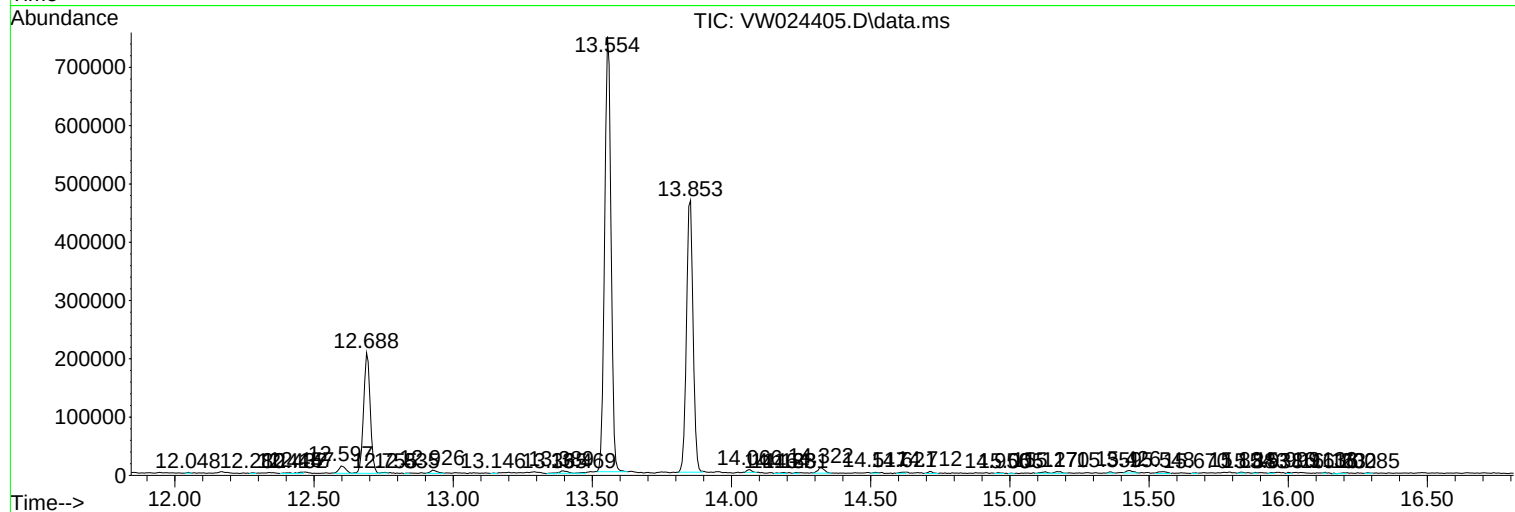
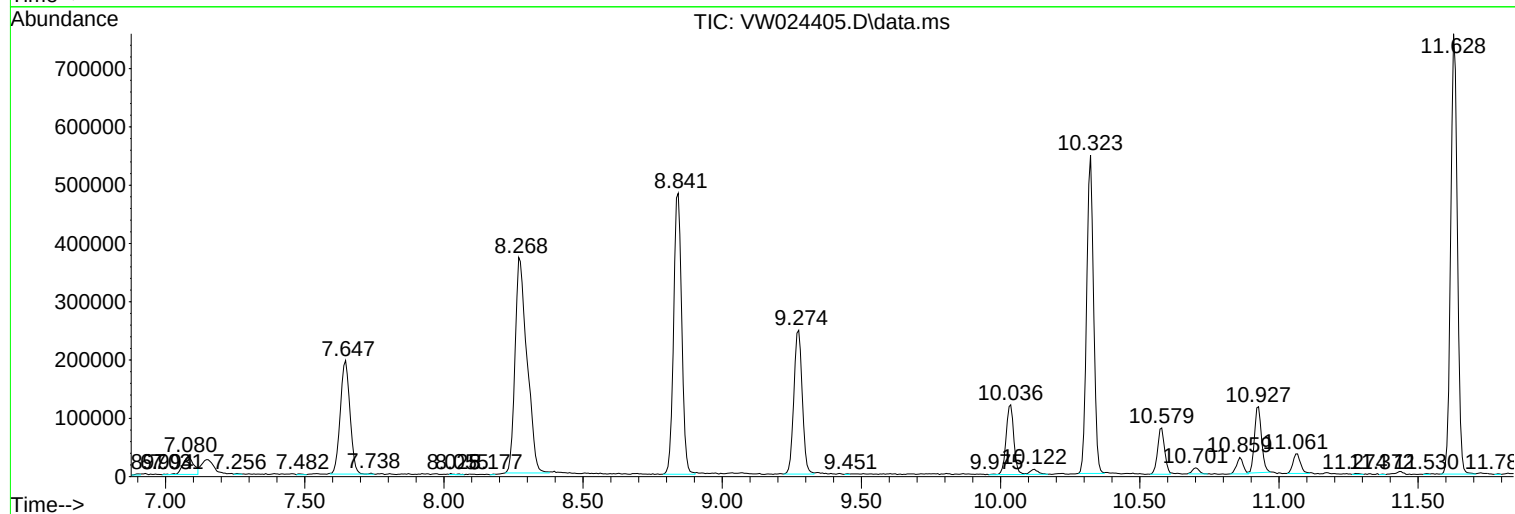
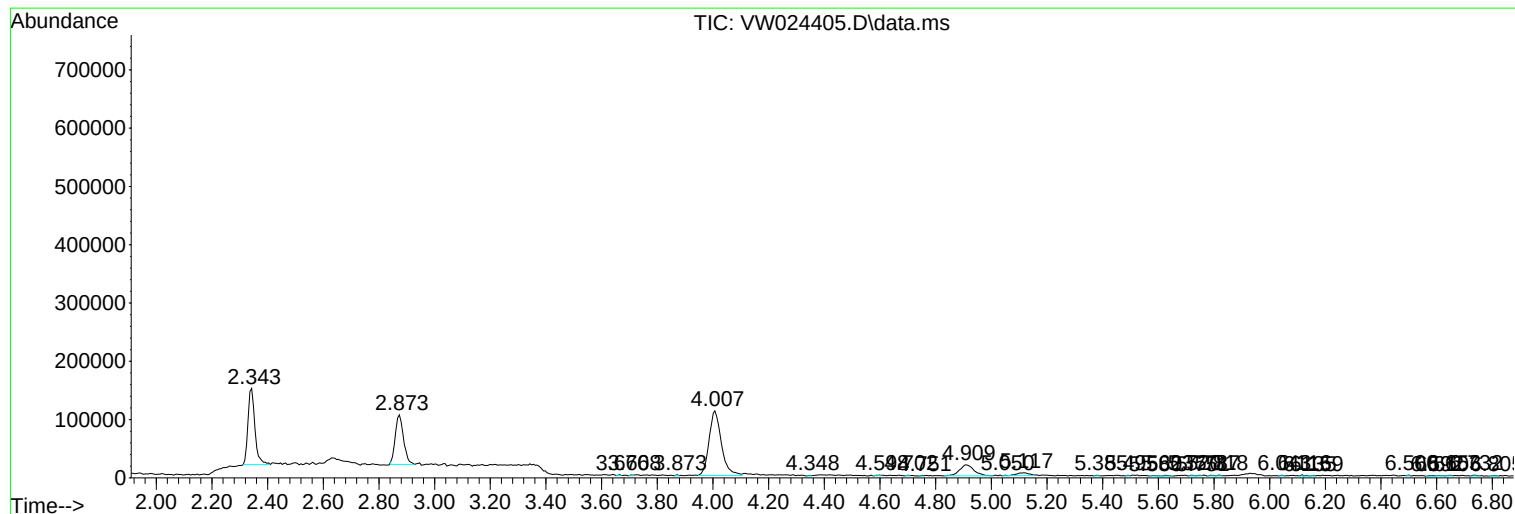
Sum of corrected areas: 9349310

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM082622SMA.M
Quant Title : SFAM01.0

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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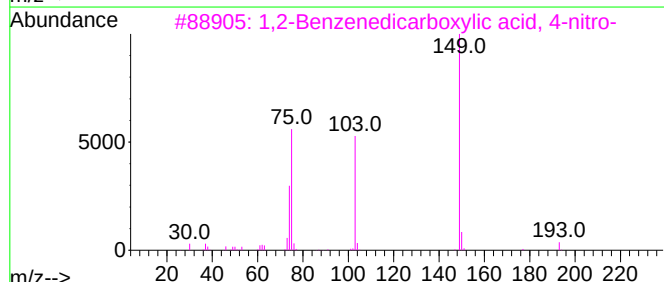
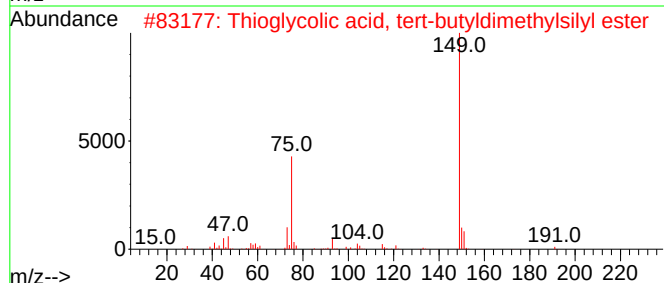
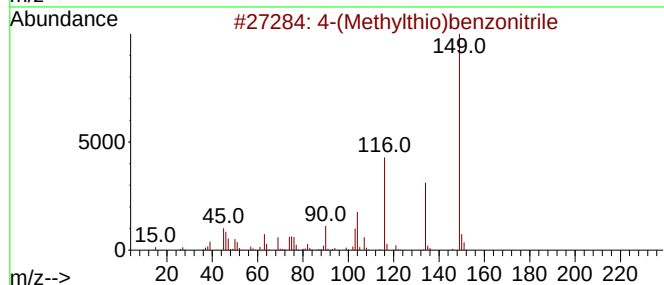
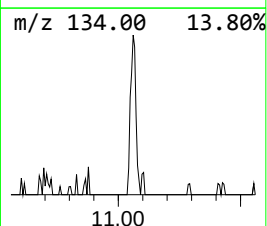
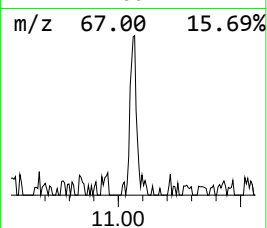
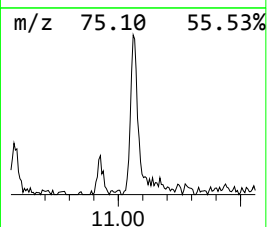
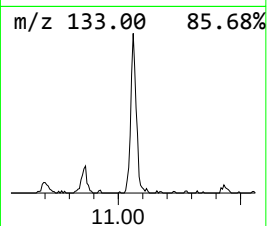
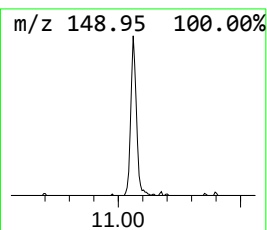
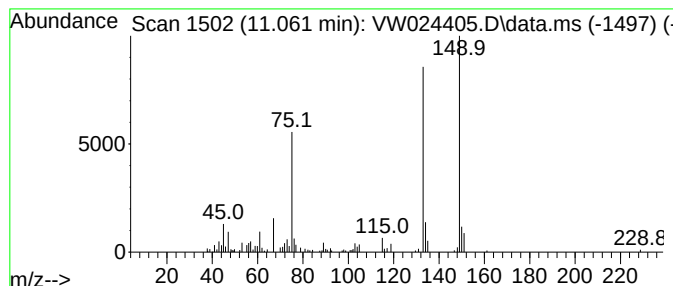
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM082622SMA.M
Quant Title : SFAM01.0

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.061	1.25 ug/L	63271	Chlorobenzene-d5	11.628

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-(Methylthio)benzonitrile	149	C8H7NS	021382-98-9	38
2			Thioglycolic acid, tert-butyldim...	206	C8H18O2SSi	1000476-01-2	37
3			1,2-Benzenedicarboxylic acid, 4-...	211	C8H5NO6	000610-27-5	32
4			4-Ethylbenzoic acid, 3-methylbut...	218	C14H18O2	1000292-54-1	27
5			Phthalic acid, propyl octadecyl ...	460	C29H48O4	1000308-96-7	22



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	11.061	1.3	ug/L	63271	2	11.628	1261850	25.0