

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW082622\
 Data File : VW024354.D
 Acq On : 26 Aug 2022 17:01
 Operator : SY/VA
 Sample : N4319-09
 Misc : 6.33g/10mL/MSVOA_W/SOIL
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 C0ZJ1

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: VW024354.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.257	47	58	61	rBV10	15769	56055	4.36%	0.559%
2	2.336	66	71	82	rVV	176838	312623	24.33%	3.120%
3	2.873	153	159	169	rVB	103062	210242	16.36%	2.098%
4	3.995	335	343	356	rBV	100137	290736	22.63%	2.901%
5	4.409	409	411	414	rVB4	1813	1599	0.12%	0.016%
6	4.513	426	428	432	rBV5	1780	1585	0.12%	0.016%
7	4.781	469	472	474	rVB4	1788	1853	0.14%	0.018%
8	4.836	477	481	482	rBV3	1990	1957	0.15%	0.020%
9	4.903	483	492	505	rVV3	27401	92425	7.19%	0.922%
10	5.037	512	514	517	rBV4	1769	2597	0.20%	0.026%
11	5.074	517	520	521	rBV3	1436	1630	0.13%	0.016%
12	5.098	521	524	525	rBV3	3205	3684	0.29%	0.037%
13	5.177	533	537	538	rBV3	2328	2447	0.19%	0.024%
14	5.196	538	540	541	rVV2	2160	1668	0.13%	0.017%
15	5.238	544	547	549	rVB4	1861	2212	0.17%	0.022%
16	5.269	549	552	555	rBV5	1030	1667	0.13%	0.017%
17	5.305	555	558	561	rBV5	1170	1683	0.13%	0.017%
18	5.409	572	575	578	rVB5	1441	1670	0.13%	0.017%
19	5.714	623	625	629	rBV5	2118	3132	0.24%	0.031%
20	5.817	640	642	646	rVB5	1410	1712	0.13%	0.017%
21	5.921	651	659	669	rBV3	9982	31813	2.48%	0.317%
22	6.055	678	681	683	rBV4	1289	1790	0.14%	0.018%
23	6.281	717	718	722	rBV3	1228	1456	0.11%	0.015%
24	6.500	750	754	756	rBV5	1201	1832	0.14%	0.018%
25	6.640	773	777	778	rVB4	1443	1523	0.12%	0.015%
26	6.805	801	804	806	rVB4	1952	2136	0.17%	0.021%
27	6.829	806	808	811	rBV4	1734	2260	0.18%	0.023%
28	6.970	828	831	832	rBV2	1662	1465	0.11%	0.015%
29	7.079	840	849	855	rVV2	29428	83803	6.52%	0.836%
30	7.159	855	862	873	rVB	40527	116884	9.10%	1.166%
31	7.329	888	890	892	rBV3	1682	1841	0.14%	0.018%
32	7.640	931	941	952	rBV	217384	527090	41.02%	5.260%
33	8.097	1015	1016	1019	rBV3	1606	1586	0.12%	0.016%
34	8.177	1028	1029	1033	rBV4	1450	1912	0.15%	0.019%
35	8.268	1033	1044	1062	rBV2	433509	1284999	100.00%	12.823%
36	8.695	1111	1114	1116	rVB4	1687	2044	0.16%	0.020%

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 Title : SFAM01.0

37	8.762	1124	1125	1128	rVB3	1871	1533	0.12%	0.015%
38	8.835	1128	1137	1148	rBV	483642	941836	73.29%	9.399%
39	9.067	1173	1175	1177	rVV2	2588	2516	0.20%	0.025%
40	9.268	1197	1208	1219	rBV	283224	578993	45.06%	5.778%
41	9.597	1260	1262	1267	rVV6	2259	4685	0.36%	0.047%
42	9.634	1267	1268	1270	rVV2	2451	2217	0.17%	0.022%
43	9.768	1286	1290	1291	rBV4	1720	1485	0.12%	0.015%
44	9.847	1299	1303	1304	rBV4	1834	2382	0.19%	0.024%
45	10.030	1321	1333	1342	rBV	135417	261667	20.36%	2.611%
46	10.115	1342	1347	1355	rVB7	4646	12161	0.95%	0.121%
47	10.323	1371	1381	1390	rBV	575226	1013811	78.90%	10.117%
48	10.499	1408	1410	1411	rVV2	1739	1551	0.12%	0.015%
49	10.573	1415	1422	1432	rVV	88709	162906	12.68%	1.626%
50	10.707	1438	1444	1450	rVB2	13522	26018	2.02%	0.260%
51	10.829	1459	1464	1466	rBV6	1872	2987	0.23%	0.030%
52	10.920	1473	1479	1490	rBV	126010	230354	17.93%	2.299%
53	11.060	1497	1502	1509	rVB2	20499	38581	3.00%	0.385%
54	11.432	1558	1563	1569	rVB4	7353	13618	1.06%	0.136%
55	11.627	1587	1595	1605	rBV	742610	1237172	96.28%	12.346%
56	11.810	1622	1625	1629	rBV6	1309	2522	0.20%	0.025%
57	12.066	1666	1667	1671	rBV4	2589	3271	0.25%	0.033%
58	12.158	1676	1682	1683	rBV6	2973	4501	0.35%	0.045%
59	12.322	1706	1709	1711	rVV4	1800	1673	0.13%	0.017%
60	12.359	1713	1715	1720	rVB6	1820	2428	0.19%	0.024%
61	12.603	1749	1755	1761	rVB3	11241	20983	1.63%	0.209%
62	12.688	1761	1769	1777	rBV	233367	387436	30.15%	3.866%
63	12.883	1795	1801	1805	rBV8	3429	6724	0.52%	0.067%
64	12.926	1805	1808	1812	rVV6	2776	3634	0.28%	0.036%
65	13.023	1819	1824	1825	rBV5	2075	2777	0.22%	0.028%
66	13.072	1828	1832	1836	rVB7	1789	3042	0.24%	0.030%
67	13.182	1845	1850	1852	rBV6	2187	3510	0.27%	0.035%
68	13.292	1863	1868	1871	rVB7	2184	3745	0.29%	0.037%
69	13.389	1881	1884	1886	rBV4	2205	2480	0.19%	0.025%
70	13.493	1899	1901	1904	rVV4	3616	4180	0.33%	0.042%
71	13.554	1904	1911	1920	rVV	658401	1026618	79.89%	10.245%
72	13.645	1922	1926	1930	rVV4	11589	17690	1.38%	0.177%
73	13.852	1952	1960	1969	rBV	486741	836158	65.07%	8.344%
74	14.005	1983	1985	1991	rVB6	2037	3460	0.27%	0.035%
75	14.060	1991	1994	2000	rBV4	3665	6569	0.51%	0.066%
76	14.243	2022	2024	2029	rBV6	1790	2270	0.18%	0.023%

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 Title : SFAM01.0

77	14.322	2032	2037	2041	rVB8	4099	6886	0.54%	0.069%
78	14.371	2043	2045	2051	rBV7	1174	2099	0.16%	0.021%
79	14.523	2066	2070	2072	rBV5	1818	2743	0.21%	0.027%
80	14.627	2082	2087	2092	rVB5	7632	12741	0.99%	0.127%
81	14.712	2099	2101	2103	rBV2	2464	3209	0.25%	0.032%
82	15.127	2165	2169	2173	rVV7	4055	6116	0.48%	0.061%
83	15.169	2174	2176	2181	rVV6	3106	4413	0.34%	0.044%
84	15.310	2195	2199	2202	rVB6	1262	1965	0.15%	0.020%
85	15.358	2204	2207	2209	rBV4	3352	4185	0.33%	0.042%
86	15.383	2209	2211	2214	rVV4	1991	1732	0.13%	0.017%
87	15.419	2214	2217	2219	rVV4	1713	2151	0.17%	0.021%
88	15.547	2235	2238	2242	rVV6	2710	4396	0.34%	0.044%
89	15.657	2251	2256	2260	rBV8	2120	3468	0.27%	0.035%
90	15.748	2266	2271	2272	rBV5	1679	2749	0.21%	0.027%
91	15.803	2276	2280	2281	rBV4	1691	1955	0.15%	0.020%
92	15.877	2290	2292	2296	rBV4	1205	1507	0.12%	0.015%
93	15.968	2305	2307	2309	rVV3	1927	2063	0.16%	0.021%
94	15.992	2309	2311	2313	rVV3	2011	1674	0.13%	0.017%
95	16.029	2315	2317	2322	rVV5	1563	2713	0.21%	0.027%
96	16.066	2322	2323	2326	rVV3	1769	1664	0.13%	0.017%
97	16.309	2358	2363	2364	rBV5	1773	2498	0.19%	0.025%
98	16.450	2382	2386	2389	rBV6	1479	2793	0.22%	0.028%
99	16.529	2395	2399	2403	rBV7	1552	2575	0.20%	0.026%
100	16.681	2421	2424	2429	rBV7	1476	3023	0.24%	0.030%

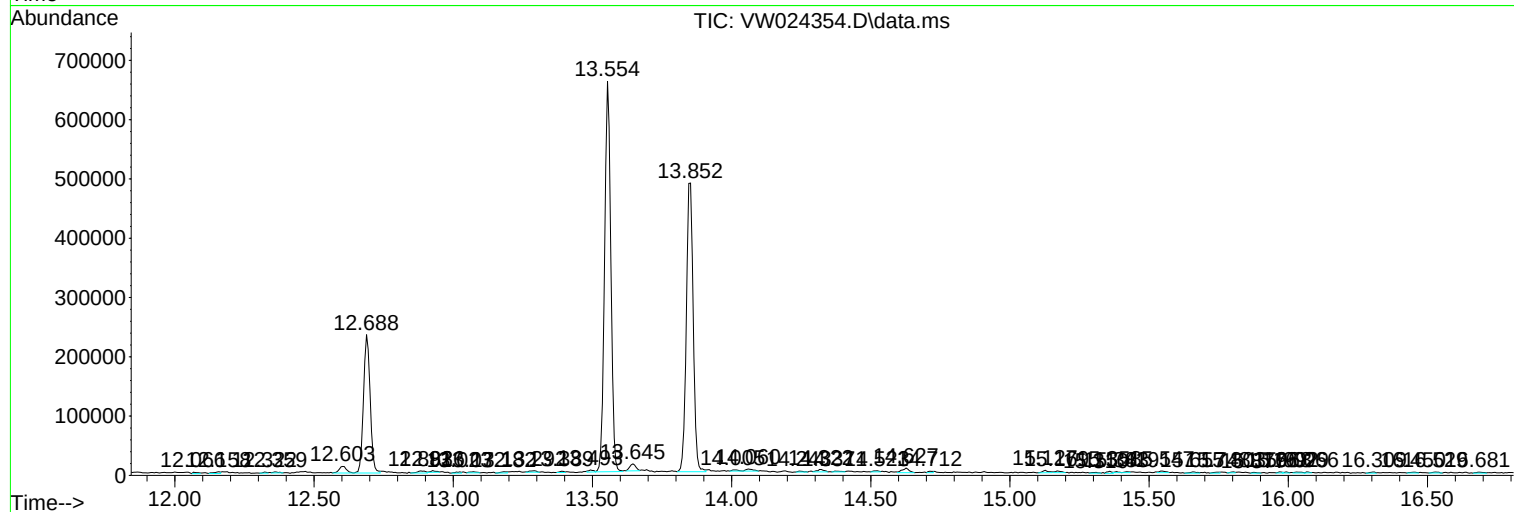
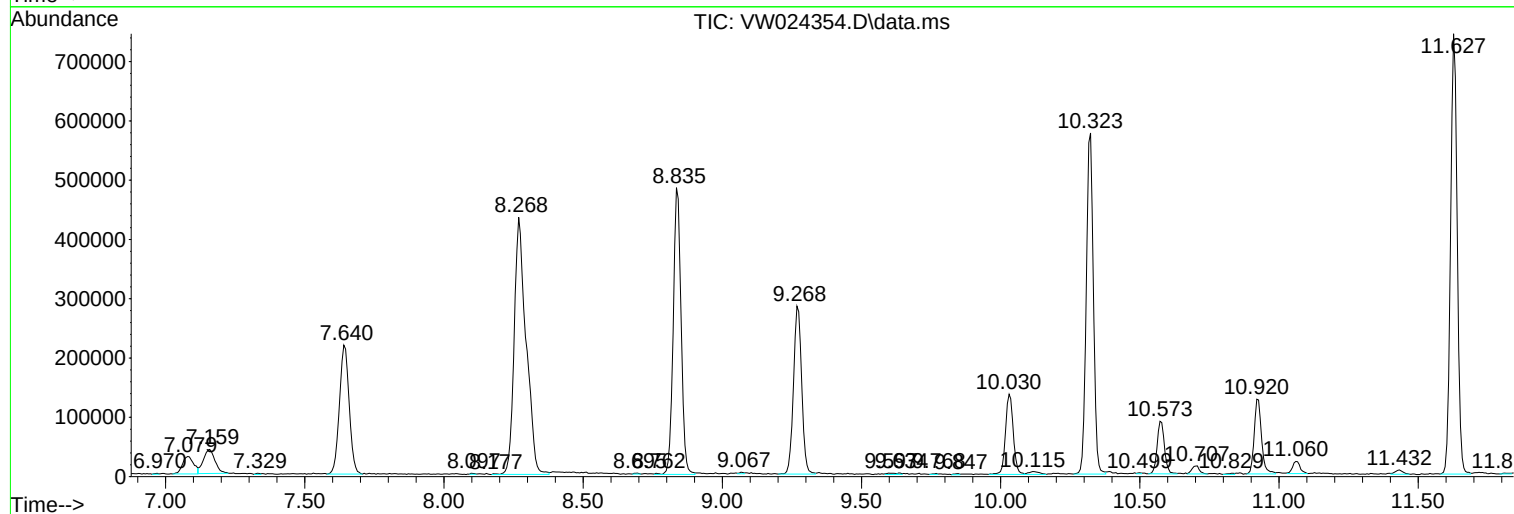
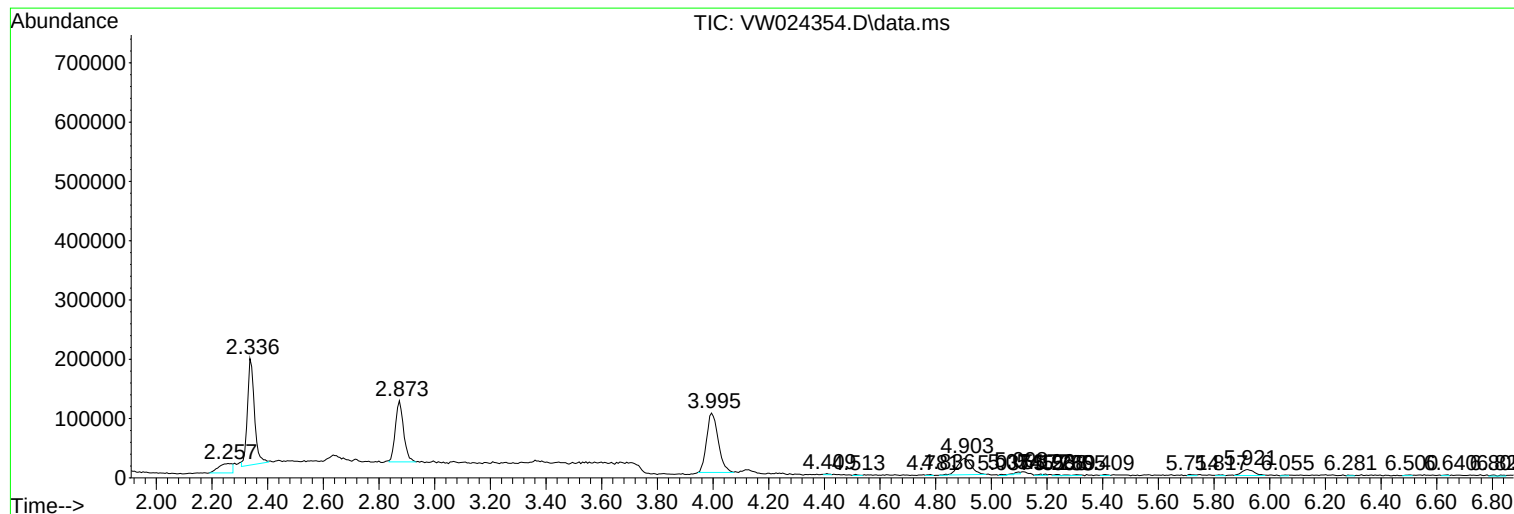
Sum of corrected areas: 10021073

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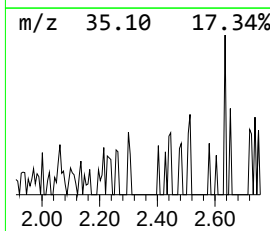
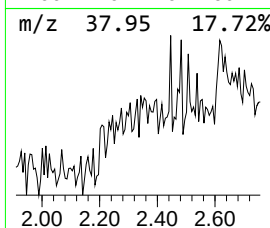
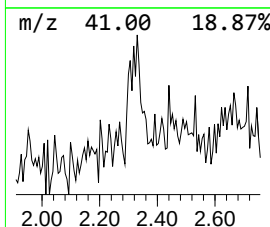
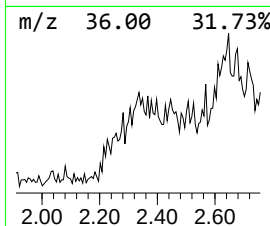
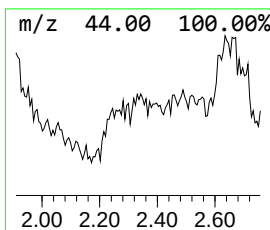
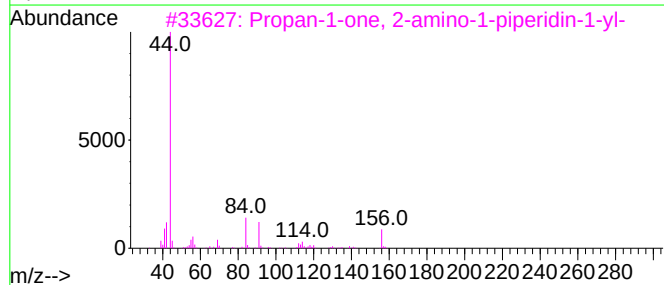
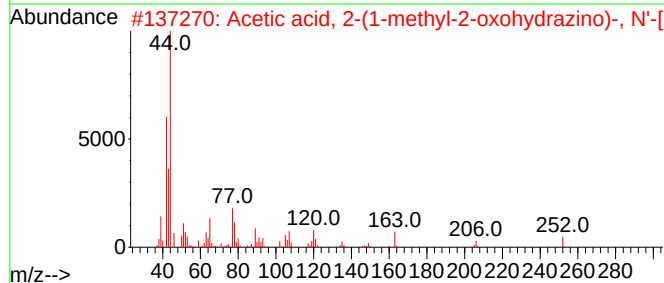
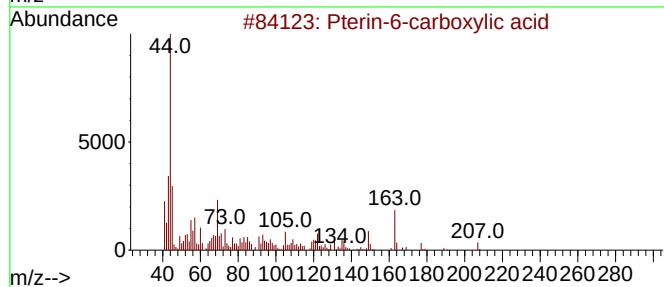
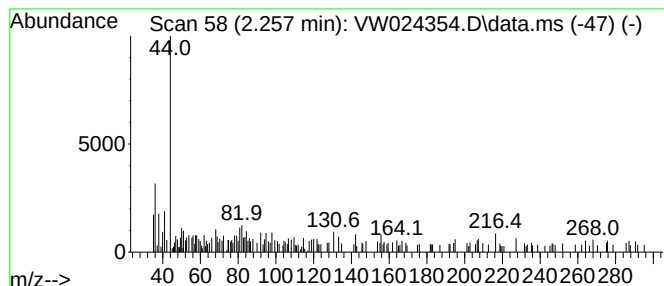
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM082622SMA.M
Quant Title : SFAM01.0

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

Peak Number 1 Pterin-6-carboxylic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.257	1.49 ug/L	56055	1,4-Difluorobenzene	8.835

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pterin-6-carboxylic acid	207	C7H5N5O3	000948-60-7	50
2			Acetic acid, 2-(1-methyl-2-oxohy...	252	C10H12N4O4	1000327-59-6	43
3			Propan-1-one, 2-amino-1-piperidi...	156	C8H16N2O	1000305-79-9	38
4			N-[3-(4-Fluorophenoxy)propyl]-N-...	183	C10H14FNO	883542-69-6	38
5			Acetamide, 2,2,2-trichloro-	161	C2H2Cl3NO	000594-65-0	38



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Pterin-6-carbox...	2.257	1.5	ug/L	56055	1	8.835	941836	25.0