

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW071322\
 Data File : VW023655.D
 Acq On : 13 Jul 2022 18:29
 Operator : SY/VA
 Sample : N3676-02RE
 Misc : 6.77g/10mL/MSVOA_W/SOIL
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 F5B01RE

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\SFAMWLM071322SMA.M
 Title : SFAM01.0

Signal : TIC: VW023655.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.251	48	57	59	rBV5	11843	34374	4.73%	0.656%
2	2.343	67	72	79	rBV	96454	155239	21.37%	2.961%
3	3.525	264	266	267	rBV2	1370	1070	0.15%	0.020%
4	3.763	303	305	307	rBV3	1025	1413	0.19%	0.027%
5	3.806	309	312	315	rBV5	1369	1683	0.23%	0.032%
6	3.873	321	323	326	rBV4	887	1269	0.17%	0.024%
7	4.013	334	346	357	rBV	56212	178316	24.55%	3.401%
8	4.854	482	484	485	rBV2	1532	1354	0.19%	0.026%
9	4.915	485	494	503	rVV4	10009	32804	4.52%	0.626%
10	5.050	514	516	517	rBV2	1645	1495	0.21%	0.029%
11	5.269	550	552	556	rVB5	1813	2252	0.31%	0.043%
12	5.318	556	560	563	rBV6	1588	3082	0.42%	0.059%
13	5.373	566	569	573	rVB6	1529	2065	0.28%	0.039%
14	5.427	577	578	581	rBV3	1143	1178	0.16%	0.022%
15	5.476	584	586	588	rBV3	912	921	0.13%	0.018%
16	5.885	651	653	654	rBV2	1121	970	0.13%	0.019%
17	6.190	701	703	707	rVV3	1113	1078	0.15%	0.021%
18	6.232	707	710	712	rVB4	1659	1523	0.21%	0.029%
19	6.257	712	714	718	rVB3	960	1089	0.15%	0.021%
20	6.299	718	721	723	rBV4	1241	1463	0.20%	0.028%
21	6.409	736	739	744	rBV7	1035	1656	0.23%	0.032%
22	6.458	744	747	750	rBV4	1155	1388	0.19%	0.026%
23	6.635	775	776	778	rBV2	1189	917	0.13%	0.017%
24	6.738	790	793	796	rBV4	1275	1309	0.18%	0.025%
25	7.000	833	836	837	rBV3	1490	1081	0.15%	0.021%
26	7.080	841	849	854	rBV	28549	72576	9.99%	1.384%
27	7.336	889	891	894	rBV4	1292	1295	0.18%	0.025%
28	7.580	929	931	932	rBV2	1322	1109	0.15%	0.021%
29	7.647	934	942	956	rVB	126054	307825	42.37%	5.872%
30	7.829	968	972	974	rBV5	1982	2824	0.39%	0.054%
31	7.860	974	977	980	rVV5	1246	1841	0.25%	0.035%
32	7.921	985	987	988	rBV2	1108	845	0.12%	0.016%
33	7.988	996	998	1000	rVB3	1479	936	0.13%	0.018%
34	8.110	1014	1018	1019	rBV4	1285	1310	0.18%	0.025%
35	8.275	1033	1045	1059	rBV2	229029	726433	100.00%	13.857%
36	8.579	1093	1095	1097	rBV3	1119	926	0.13%	0.018%

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Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM071322SMA.M
 Title : SFAM01.0

37	8.604	1097	1099	1105	rVB7	2193	3407	0.47%	0.065%
38	8.659	1105	1108	1110	rBV4	1349	1757	0.24%	0.034%
39	8.689	1110	1113	1114	rBV3	1542	1728	0.24%	0.033%
40	8.841	1128	1138	1148	rBV	236240	450518	62.02%	8.594%
41	9.207	1196	1198	1200	rBV3	1451	1174	0.16%	0.022%
42	9.274	1201	1209	1218	rVV	163609	327352	45.06%	6.244%
43	9.555	1254	1255	1257	rVB2	1432	886	0.12%	0.017%
44	9.579	1257	1259	1260	rBV2	1061	1024	0.14%	0.020%
45	9.604	1260	1263	1265	rVV4	1321	1417	0.20%	0.027%
46	9.665	1268	1273	1277	rVV7	2765	4717	0.65%	0.090%
47	9.725	1282	1283	1286	rBV3	1179	1067	0.15%	0.020%
48	9.866	1304	1306	1307	rBV2	1624	1287	0.18%	0.025%
49	10.036	1327	1334	1342	rVB	72947	133731	18.41%	2.551%
50	10.122	1344	1348	1351	rBV6	2721	4450	0.61%	0.085%
51	10.323	1373	1381	1388	rBV	315774	539486	74.27%	10.291%
52	10.579	1416	1423	1432	rBV2	51011	95939	13.21%	1.830%
53	10.701	1437	1443	1448	rVB4	10766	19537	2.69%	0.373%
54	10.853	1463	1468	1473	rBV8	3490	6451	0.89%	0.123%
55	10.926	1473	1480	1493	rVB	121001	216713	29.83%	4.134%
56	11.024	1493	1496	1497	rBV3	1837	1848	0.25%	0.035%
57	11.061	1497	1502	1512	rVB	29674	52821	7.27%	1.008%
58	11.176	1517	1521	1524	rBV6	2560	4249	0.58%	0.081%
59	11.274	1534	1537	1541	rVB5	1058	1263	0.17%	0.024%
60	11.433	1559	1563	1569	rVB3	7519	13495	1.86%	0.257%
61	11.512	1572	1576	1578	rBV5	1781	2146	0.30%	0.041%
62	11.628	1586	1595	1605	rBV	319553	545190	75.05%	10.400%
63	11.798	1621	1623	1625	rBV3	1077	876	0.12%	0.017%
64	12.067	1663	1667	1670	rBV5	1848	3433	0.47%	0.065%
65	12.341	1709	1712	1713	rBV3	893	836	0.12%	0.016%
66	12.432	1724	1727	1730	rVB4	1088	1273	0.18%	0.024%
67	12.463	1730	1732	1737	rBV5	2201	3294	0.45%	0.063%
68	12.603	1750	1755	1761	rVB5	10979	21133	2.91%	0.403%
69	12.688	1763	1769	1777	rVV	168025	281294	38.72%	5.366%
70	12.847	1794	1795	1799	rVV4	1250	1470	0.20%	0.028%
71	12.932	1805	1809	1818	rVB7	6619	13060	1.80%	0.249%
72	13.072	1826	1832	1833	rBV5	1471	2673	0.37%	0.051%
73	13.115	1837	1839	1841	rVV3	1412	1063	0.15%	0.020%
74	13.188	1844	1851	1856	rBV6	4820	10210	1.41%	0.195%
75	13.408	1879	1887	1892	rVB8	6553	13180	1.81%	0.251%
76	13.499	1899	1902	1903	rBV3	1769	1620	0.22%	0.031%

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Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM071322SMA.M
 Title : SFAM01.0

77	13.554	1905	1911	1917	rBV	265254	435607	59.97%	8.309%
78	13.853	1953	1960	1967	rBV	249829	419007	57.68%	7.993%
79	14.066	1992	1995	2005	rVB7	5540	14872	2.05%	0.284%
80	14.188	2011	2015	2017	rBV4	1657	2100	0.29%	0.040%
81	14.481	2060	2063	2064	rBV3	1524	1635	0.23%	0.031%
82	14.584	2078	2080	2082	rBV3	913	946	0.13%	0.018%
83	14.621	2084	2086	2088	rBV3	1734	1922	0.26%	0.037%
84	14.712	2099	2101	2105	rVB4	4785	6093	0.84%	0.116%
85	14.840	2120	2122	2126	rBV5	1072	1227	0.17%	0.023%
86	15.029	2150	2153	2154	rBV3	1033	882	0.12%	0.017%
87	15.121	2166	2168	2171	rBV4	1701	2194	0.30%	0.042%
88	15.353	2204	2206	2209	rVB4	1502	1613	0.22%	0.031%
89	15.383	2209	2211	2212	rBV2	1375	1273	0.18%	0.024%
90	15.548	2234	2238	2243	rBV9	1439	3000	0.41%	0.057%
91	15.633	2250	2252	2254	rBV3	1036	1018	0.14%	0.019%
92	15.822	2281	2283	2285	rBV3	1006	1264	0.17%	0.024%
93	16.072	2322	2324	2327	rBV4	904	1111	0.15%	0.021%
94	16.200	2342	2345	2349	rVB5	939	1147	0.16%	0.022%
95	16.230	2349	2350	2353	rBV2	907	908	0.12%	0.017%
96	16.352	2367	2370	2371	rBV2	1328	1333	0.18%	0.025%
97	16.456	2384	2387	2389	rBV4	1291	1452	0.20%	0.028%
98	16.554	2400	2403	2405	rVB4	960	1151	0.16%	0.022%
99	16.584	2405	2408	2409	rBV3	1207	1496	0.21%	0.029%
100	16.627	2413	2415	2416	rBV2	1393	1163	0.16%	0.022%

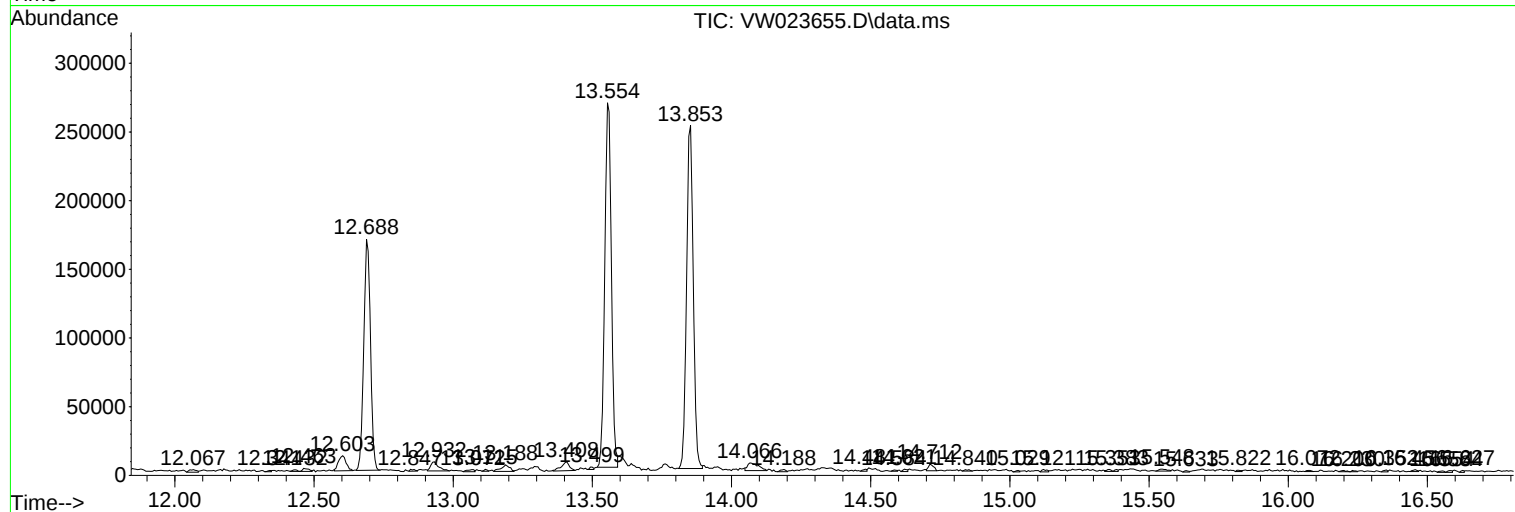
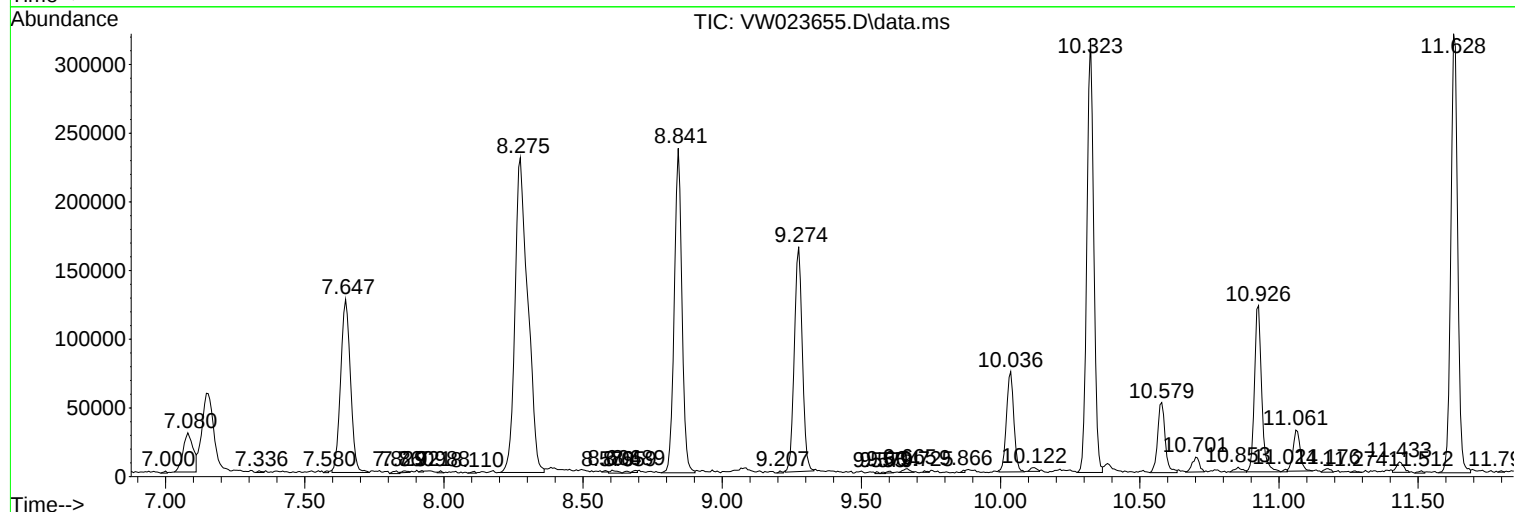
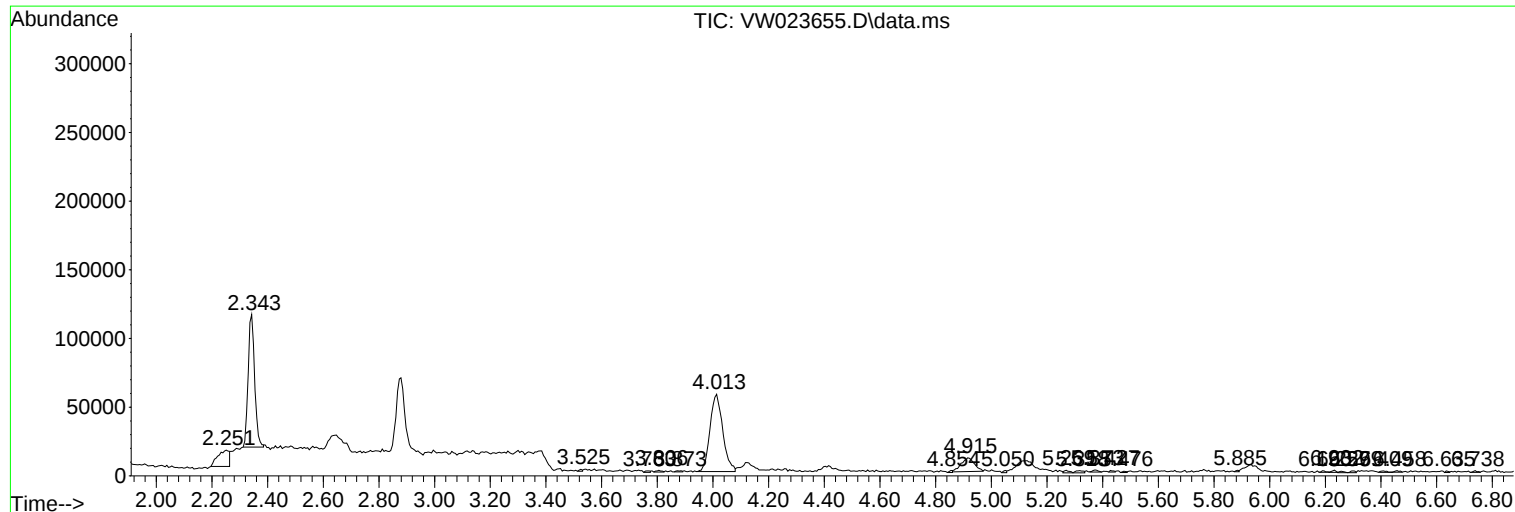
Sum of corrected areas: 5242391

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Instrument :
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM071322SMA.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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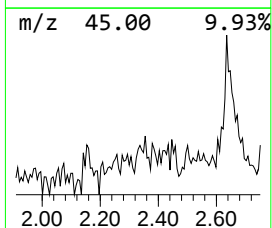
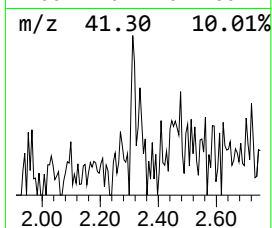
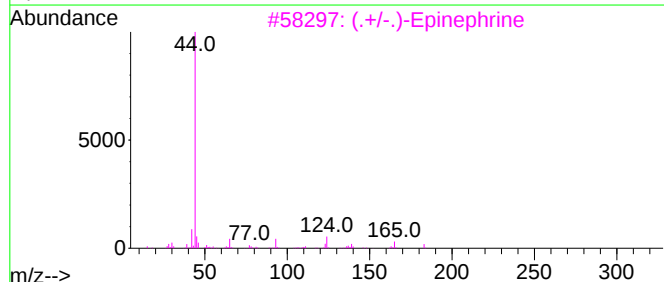
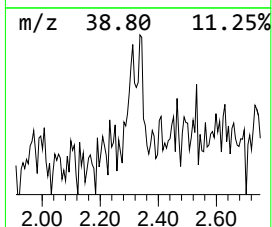
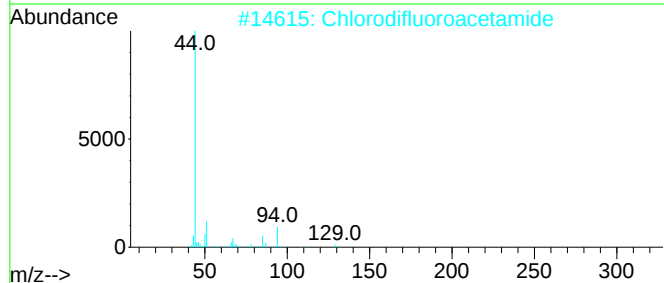
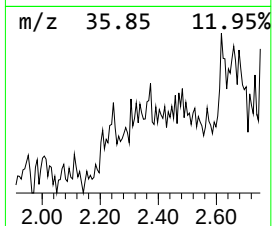
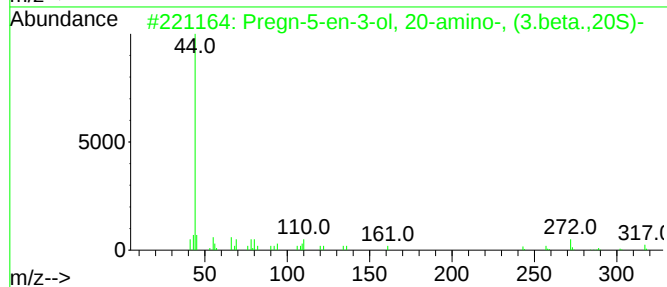
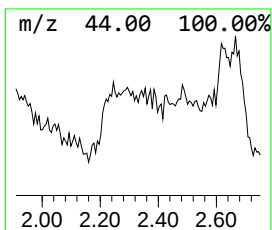
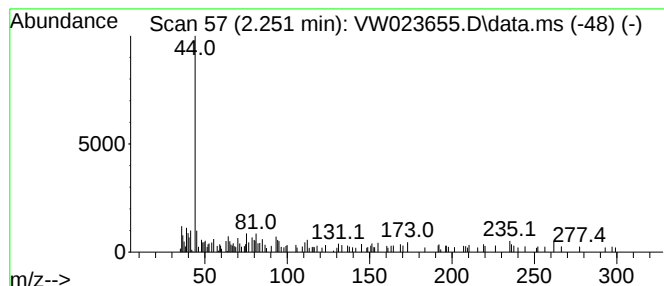
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM071322SMA.M
Quant Title : SFAM01.0

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

Peak Number 1 Pregn-5-en-3-ol, 20-amino-,... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.251	1.91 ug/L	34374	1,4-Difluorobenzene	8.841

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pregn-5-en-3-ol, 20-amino-, (3.b...	317	C21H35NO	005035-10-9	50
2			Chlorodifluoroacetamide	129	C2H2ClF2NO	000354-28-9	47
3			(.+/-)-Epinephrine	183	C9H13NO3	000329-65-7	43
4			1,5,2,4-Dioxadithiepane-2,2,4,4-...	202	C3H6O6S2	099591-73-8	42
5			Pterin-6-carboxylic acid	207	C7H5N5O3	000948-60-7	42



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Pregn-5-en-3-ol...	2.251	1.9	ug/L	34374	1	8.841	450518	25.0