

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW071322\
 Data File : VW023650.D
 Acq On : 13 Jul 2022 16:25
 Operator : SY/VA
 Sample : VIBLK508
 Misc : 5.00g/10mL/MSVOA_W/SOIL
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 VIBLK508

Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : OFF
 Sampling : 1
 Start Thrs : 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 0 % 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\SFAMWLM071322SMA.M
 Title : SFAM01.0

Signal : TIC: VW023650.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.245	48	56	58	rBV3	11958	30878	3.86%	0.486%
2	2.343	68	72	81	rVB	127442	220715	27.62%	3.477%
3	2.879	156	160	170	rVB	70899	152580	19.09%	2.404%
4	3.568	271	273	276	rVB3	1525	1379	0.17%	0.022%
5	4.013	333	346	364	rBV3	65230	229779	28.75%	3.620%
6	4.391	406	408	410	rBV3	1661	1734	0.22%	0.027%
7	4.605	441	443	446	rBV4	845	989	0.12%	0.016%
8	4.733	461	464	465	rBV2	1585	1585	0.20%	0.025%
9	4.861	481	485	486	rBV4	1509	2011	0.25%	0.032%
10	4.922	486	495	506	rVV4	9321	35639	4.46%	0.561%
11	5.098	521	524	525	rBV3	3053	3147	0.39%	0.050%
12	5.440	576	580	583	rBV6	1137	1558	0.19%	0.025%
13	5.726	625	627	629	rBV3	1252	1473	0.18%	0.023%
14	5.927	650	660	667	rBV10	6181	21159	2.65%	0.333%
15	6.226	707	709	713	rVB4	1304	1746	0.22%	0.028%
16	6.257	713	714	717	rBV3	905	981	0.12%	0.015%
17	6.281	717	718	721	rBV3	1325	1444	0.18%	0.023%
18	6.494	750	753	754	rVB3	982	989	0.12%	0.016%
19	6.842	807	810	813	rVB4	1031	1008	0.13%	0.016%
20	6.897	817	819	822	rBV4	1531	1905	0.24%	0.030%
21	7.074	841	848	855	rBV2	22998	66763	8.35%	1.052%
22	7.415	902	904	905	rBV	1329	994	0.12%	0.016%
23	7.647	933	942	952	rBV2	130992	321688	40.25%	5.068%
24	7.872	976	979	981	rBV3	1236	1595	0.20%	0.025%
25	8.092	1011	1015	1018	rVB6	1155	1758	0.22%	0.028%
26	8.275	1034	1045	1058	rVV2	256111	799233	100.00%	12.590%
27	8.659	1106	1108	1110	rBV3	1280	1237	0.15%	0.019%
28	8.842	1130	1138	1147	rBV2	246696	481284	60.22%	7.582%
29	8.988	1160	1162	1164	rBV3	1360	1297	0.16%	0.020%
30	9.274	1200	1209	1218	rVV	172021	356410	44.59%	5.614%
31	9.506	1245	1247	1251	rVB5	1467	1469	0.18%	0.023%
32	9.537	1251	1252	1257	rBV5	1605	1875	0.23%	0.030%
33	9.591	1257	1261	1265	rBV7	1791	3071	0.38%	0.048%
34	9.762	1287	1289	1290	rBV2	1284	1313	0.16%	0.021%
35	9.817	1296	1298	1300	rBV3	1605	1381	0.17%	0.022%
36	9.866	1302	1306	1307	rBV4	1204	1315	0.16%	0.021%

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 ClientSampleId :
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Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : OFF
 Sampling : 1
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 Stop Thrs : 0

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 Peak Location: TOP

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

37	10.036	1318	1334	1342	rBV	92321	177233	22.18%	2.792%
38	10.201	1359	1361	1365	rBV4	1495	1763	0.22%	0.028%
39	10.323	1373	1381	1393	rBV	374333	644859	80.68%	10.158%
40	10.463	1403	1404	1407	rVB3	1778	960	0.12%	0.015%
41	10.512	1410	1412	1413	rBV2	1353	1143	0.14%	0.018%
42	10.579	1416	1423	1429	rBV	62650	110135	13.78%	1.735%
43	10.701	1437	1443	1451	rVB	62605	113662	14.22%	1.791%
44	10.847	1460	1467	1471	rBV10	4080	7854	0.98%	0.124%
45	10.927	1473	1480	1488	rBV	103320	174405	21.82%	2.747%
46	11.061	1496	1502	1508	rBV	50786	83982	10.51%	1.323%
47	11.170	1516	1520	1526	rVB6	5077	9570	1.20%	0.151%
48	11.262	1533	1535	1538	rBV4	776	934	0.12%	0.015%
49	11.292	1538	1540	1542	rVB3	1228	973	0.12%	0.015%
50	11.439	1559	1564	1569	rVB	21526	36192	4.53%	0.570%
51	11.628	1588	1595	1604	rBV	374777	637410	79.75%	10.041%
52	11.792	1620	1622	1625	rBV4	1063	1364	0.17%	0.021%
53	11.829	1626	1628	1630	rVV3	1280	975	0.12%	0.015%
54	12.128	1673	1677	1679	rBV5	833	1187	0.15%	0.019%
55	12.237	1691	1695	1696	rVV4	1471	1610	0.20%	0.025%
56	12.274	1700	1701	1706	rVB4	1299	1208	0.15%	0.019%
57	12.323	1706	1709	1712	rBV4	1334	1601	0.20%	0.025%
58	12.499	1736	1738	1741	rVB4	1330	1061	0.13%	0.017%
59	12.530	1741	1743	1746	rBV4	751	1167	0.15%	0.018%
60	12.603	1749	1755	1762	rVB	35759	61313	7.67%	0.966%
61	12.688	1762	1769	1776	rBV	158476	261995	32.78%	4.127%
62	12.816	1787	1790	1793	rVB4	1217	1220	0.15%	0.019%
63	12.859	1793	1797	1799	rBV4	1271	1801	0.23%	0.028%
64	12.932	1804	1809	1813	rVV4	7120	10926	1.37%	0.172%
65	13.018	1822	1823	1825	rBV2	1808	1263	0.16%	0.020%
66	13.066	1829	1831	1837	rVB5	1714	3096	0.39%	0.049%
67	13.188	1850	1851	1853	rVV2	1327	1104	0.14%	0.017%
68	13.225	1855	1857	1860	rVV3	1981	1980	0.25%	0.031%
69	13.286	1863	1867	1872	rBV8	4424	6505	0.81%	0.102%
70	13.554	1905	1911	1919	rVV	373315	595050	74.45%	9.374%
71	13.761	1940	1945	1947	rBV6	1835	3598	0.45%	0.057%
72	13.792	1947	1950	1952	rVV3	2471	2662	0.33%	0.042%
73	13.853	1952	1960	1974	rVV	331012	555284	69.48%	8.747%
74	14.011	1983	1986	1987	rBV3	1063	1421	0.18%	0.022%
75	14.066	1990	1995	2001	rVB	13771	24235	3.03%	0.382%
76	14.182	2010	2014	2017	rBV4	1513	2627	0.33%	0.041%

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 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 VIBLK508

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

77	14.322	2032	2037	2042	rVV8	2553	5123	0.64%	0.081%
78	14.402	2048	2050	2054	rVB5	1298	1411	0.18%	0.022%
79	14.438	2054	2056	2059	rBV4	874	1345	0.17%	0.021%
80	14.493	2062	2065	2068	rBV5	1462	2122	0.27%	0.033%
81	14.627	2085	2087	2091	rVB5	2636	2678	0.34%	0.042%
82	14.664	2091	2093	2095	rVB3	1282	1027	0.13%	0.016%
83	14.688	2095	2097	2098	rBV2	1127	1083	0.14%	0.017%
84	14.798	2113	2115	2116	rVV2	1437	1023	0.13%	0.016%
85	14.834	2119	2121	2124	rVB4	958	1018	0.13%	0.016%
86	14.859	2124	2125	2128	rBV3	888	1078	0.13%	0.017%
87	14.962	2140	2142	2144	rBV3	1037	961	0.12%	0.015%
88	14.981	2144	2145	2148	rBV3	805	948	0.12%	0.015%
89	15.078	2156	2161	2162	rBV4	1289	1698	0.21%	0.027%
90	15.237	2181	2187	2188	rBV5	1174	1332	0.17%	0.021%
91	15.353	2205	2206	2211	rVB4	1724	1948	0.24%	0.031%
92	15.401	2211	2214	2215	rBV3	1685	1840	0.23%	0.029%
93	15.432	2215	2219	2223	rVB5	6685	9651	1.21%	0.152%
94	15.529	2233	2235	2236	rBV2	1512	1250	0.16%	0.020%
95	15.798	2277	2279	2281	rBV3	1338	1223	0.15%	0.019%
96	15.871	2289	2291	2296	rVB5	1526	1530	0.19%	0.024%
97	16.298	2357	2361	2362	rVB4	1317	1411	0.18%	0.022%
98	16.316	2362	2364	2366	rBV3	1423	1359	0.17%	0.021%
99	16.493	2391	2393	2395	rBV3	1238	1180	0.15%	0.019%
100	16.578	2405	2407	2409	rBV4	890	1085	0.14%	0.017%

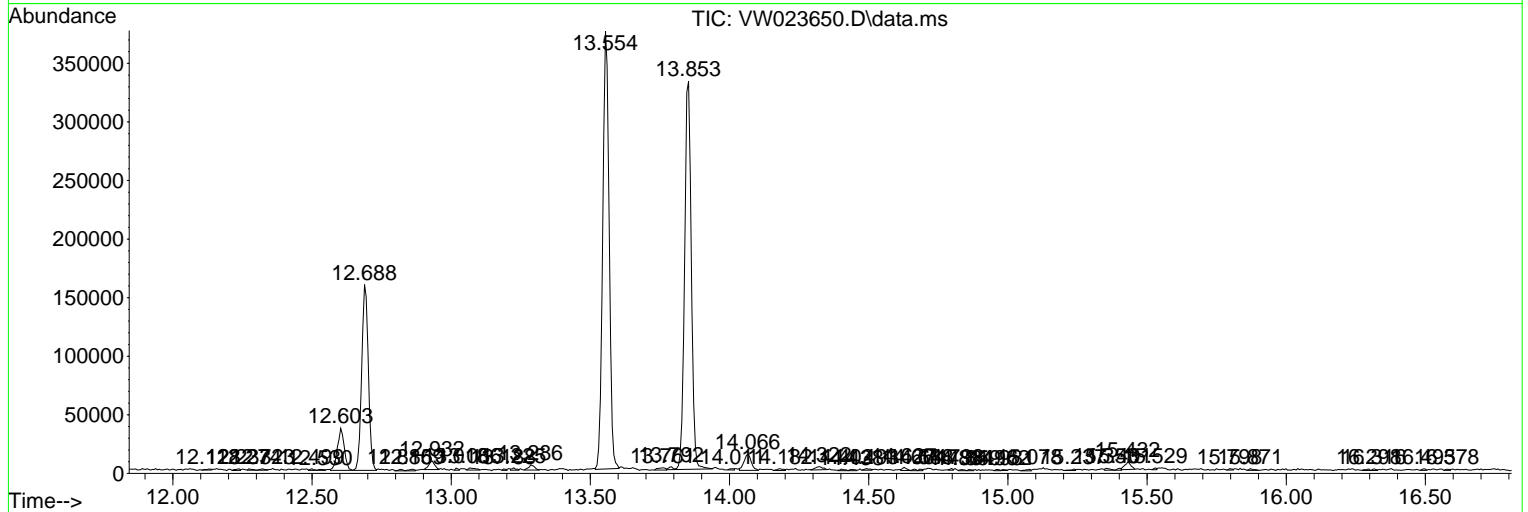
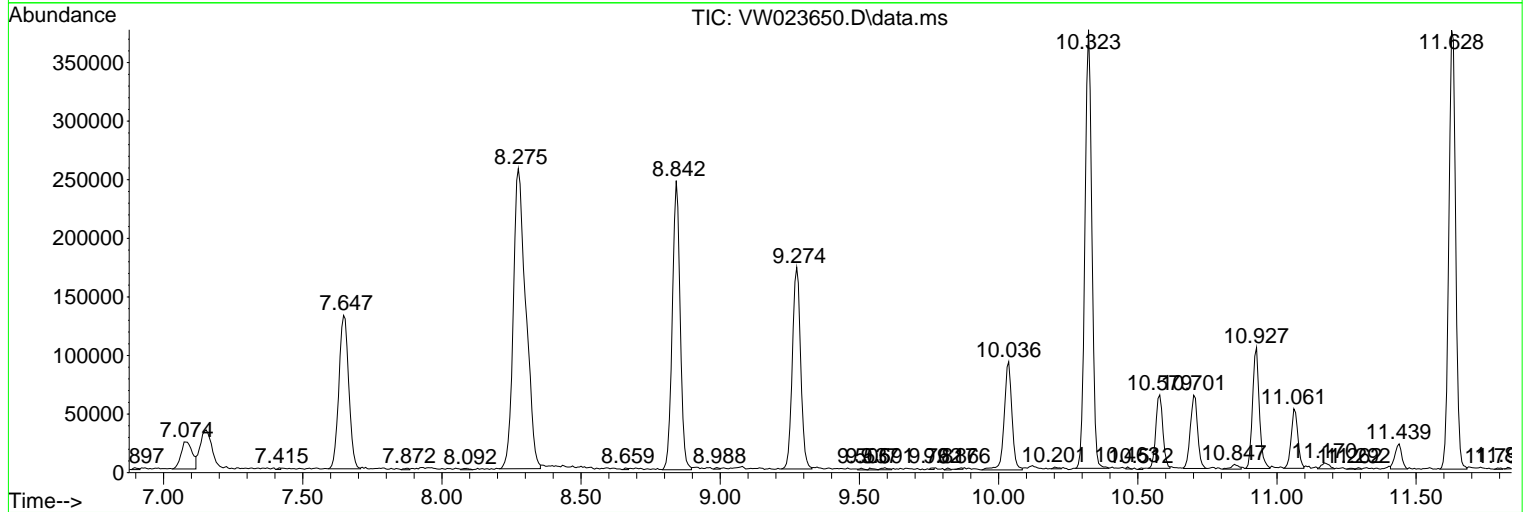
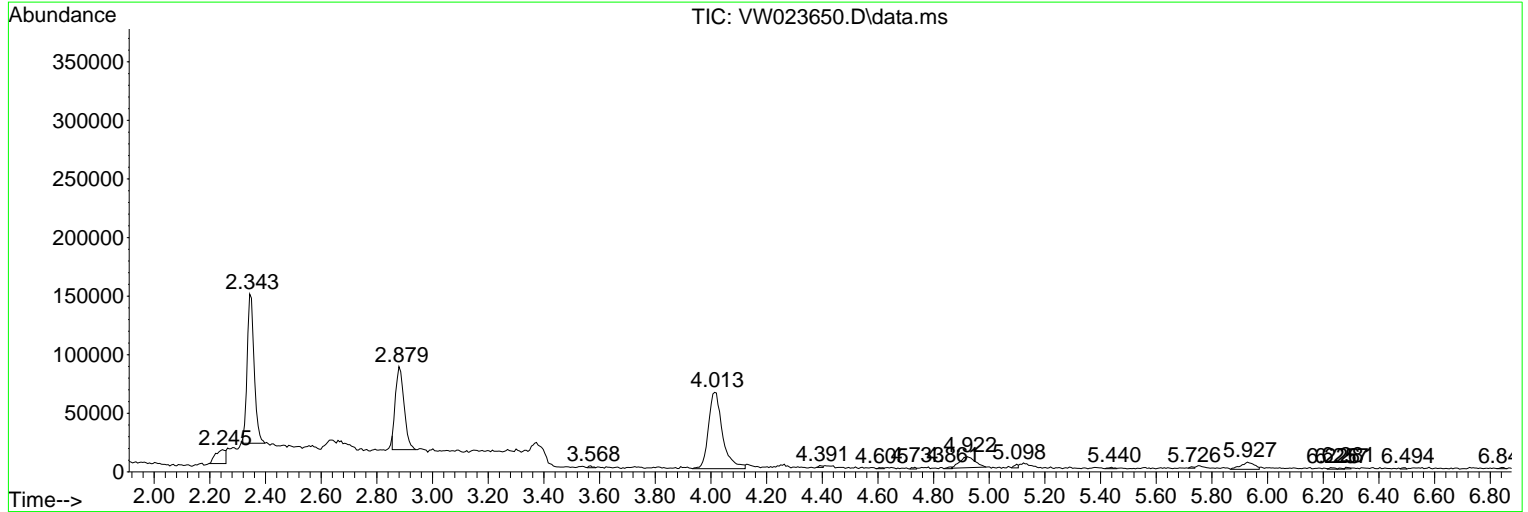
Sum of corrected areas: 6348034

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 Acq On : 13 Jul 2022 16:25
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 Misc : 5.00g/10mL/MSVOA_W/SOIL
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_W
ClientSampleId :
 VIBLK508

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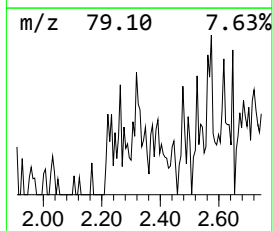
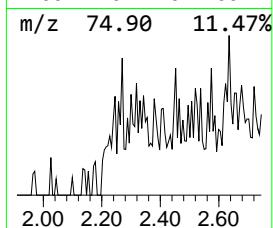
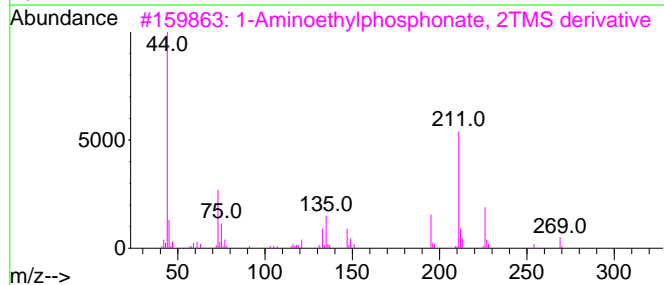
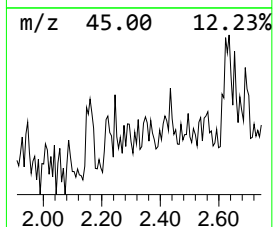
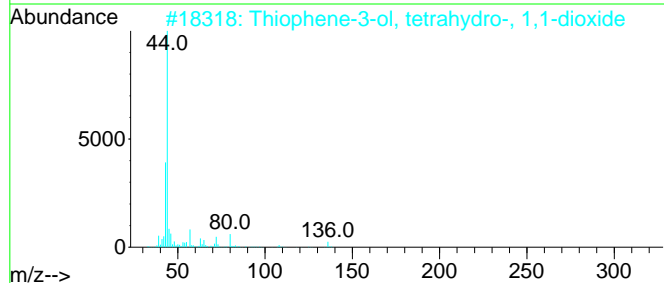
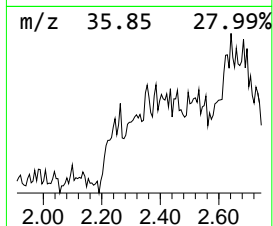
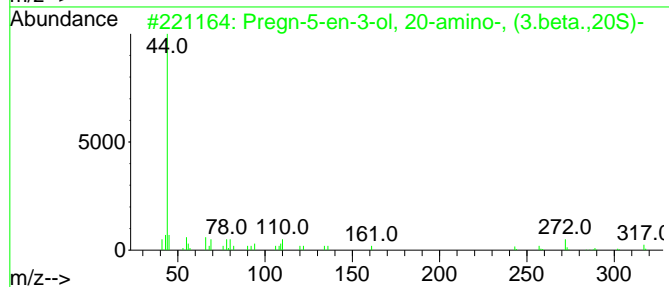
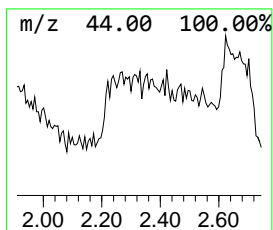
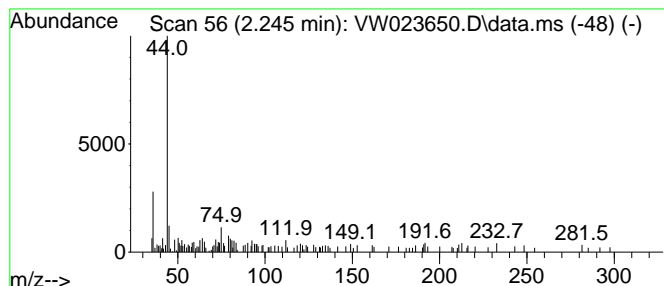
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM071322SMA.M
 Quant Title : SFAM01.0

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

 Peak Number 1 Pregn-5-en-3-ol, 20-amino-,... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.245	1.60 ug/L	30878	1,4-Difluorobenzene	8.842

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pregn-5-en-3-ol, 20-amino-, (3.b...	317	C21H35NO	005035-10-9	59
2			Thiophene-3-ol, tetrahydro-, 1,1...	136	C4H8O3S	013031-76-0	50
3			1-Aminoethylphosphonate, 2TMS de...	269	C8H24N03PSi2	053121-99-6	50
4			L-Alanine, TMS derivative	161	C6H15N02Si	1000333-28-1	47
5			Acetamide, 2,2,2-trifluoro-	113	C2H2F3NO	000354-38-1	47



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Pregn-5-en-3-ol...	2.245	1.6	ug/L	30878	1	8.842	481284	25.0