

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW121221\
 Data File : VW021344.D
 Acq On : 12 Dec 2021 02:21
 Operator : SY/VA
 Sample : M5062-13
 Misc : 6.18g/10.0mL/MSVOA_W/SOIL
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 BGL12

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\SFAMWLM120921SMA.M
 Title : SFAM01.0

Signal : TIC: VW021344.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.349	69	73	82	rVB	28671	46409	0.08%	0.043%
2	2.885	155	161	170	rVB	17317	37703	0.07%	0.035%
3	3.263	222	223	227	rVB	298	255	0.00%	0.000%
4	3.312	227	231	233	rBV5	682	1146	0.00%	0.001%
5	3.781	302	308	316	rVB2	2081	5733	0.01%	0.005%
6	3.860	319	321	325	rBV	169	251	0.00%	0.000%
7	3.952	332	336	337	rBV	278	305	0.00%	0.000%
8	4.037	337	350	377	rBV2	305535	916157	1.65%	0.845%
9	4.251	383	385	387	rVV3	236	194	0.00%	0.000%
10	4.379	399	406	417	rVB	4998	13946	0.03%	0.013%
11	4.610	443	444	448	rBV2	213	226	0.00%	0.000%
12	4.915	484	494	507	rVB3	7112	23897	0.04%	0.022%
13	5.025	509	512	514	rBV	191	214	0.00%	0.000%
14	5.128	527	529	533	rBV	189	229	0.00%	0.000%
15	5.427	568	578	588	rBV2	4944	14853	0.03%	0.014%
16	5.519	592	593	597	rBV	289	273	0.00%	0.000%
17	5.738	628	629	632	rVB2	173	184	0.00%	0.000%
18	5.793	632	638	640	rBV2	229	403	0.00%	0.000%
19	5.811	640	641	643	rVV	313	188	0.00%	0.000%
20	5.836	643	645	647	rVV	227	211	0.00%	0.000%
21	5.878	650	652	655	rBV	222	225	0.00%	0.000%
22	5.933	659	661	663	rVV	464	454	0.00%	0.000%
23	5.958	663	665	668	rVB2	438	384	0.00%	0.000%
24	6.104	687	689	691	rBV	195	203	0.00%	0.000%
25	6.220	695	708	723	rVV2	151535	467480	0.84%	0.431%
26	6.579	765	767	770	rBV	206	203	0.00%	0.000%
27	6.695	785	786	790	rVV2	166	191	0.00%	0.000%
28	7.006	835	837	841	rBV2	202	354	0.00%	0.000%
29	7.073	841	848	855	rBV	6452	17731	0.03%	0.016%
30	7.171	856	864	874	rVB	49407	128451	0.23%	0.118%
31	7.482	913	915	917	rBV	155	193	0.00%	0.000%
32	7.646	933	942	954	rVB	49293	120576	0.22%	0.111%
33	7.805	966	968	973	rVB	200	258	0.00%	0.000%
34	7.921	985	987	990	rVB	228	218	0.00%	0.000%
35	7.951	990	992	993	rBV	271	184	0.00%	0.000%
36	8.274	1036	1045	1060	rBV2	82241	262655	0.47%	0.242%

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Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM120921SMA.M
 Title : SFAM01.0

37	8.695	1110	1114	1117	rBV	193	248	0.00%	0.000%
38	8.744	1120	1122	1126	rVB2	159	209	0.00%	0.000%
39	8.841	1130	1138	1146	rVV	71024	139783	0.25%	0.129%
40	9.097	1169	1180	1202	rVV3	17524686	49013630	88.13%	45.200%
41	9.274	1202	1209	1221	rVB	55847	114053	0.21%	0.105%
42	9.475	1240	1242	1247	rVB2	302	364	0.00%	0.000%
43	9.622	1263	1266	1268	rBV3	148	228	0.00%	0.000%
44	9.756	1286	1288	1293	rVB3	400	455	0.00%	0.000%
45	9.804	1293	1296	1299	rVB3	251	264	0.00%	0.000%
46	9.835	1299	1301	1302	rBV	225	188	0.00%	0.000%
47	9.884	1304	1309	1315	rVB5	1973	3713	0.01%	0.003%
48	9.951	1319	1320	1323	rBV	179	195	0.00%	0.000%
49	10.036	1327	1334	1341	rBV2	27075	48837	0.09%	0.045%
50	10.323	1374	1381	1386	rBV	105480	183292	0.33%	0.169%
51	10.390	1386	1392	1404	rVB	477440	821670	1.48%	0.758%
52	10.493	1407	1409	1414	rVB2	331	388	0.00%	0.000%
53	10.579	1416	1423	1430	rBB	14714	25676	0.05%	0.024%
54	10.701	1438	1443	1448	rBV3	546	1187	0.00%	0.001%
55	10.756	1449	1452	1457	rVB2	1049	1411	0.00%	0.001%
56	10.871	1461	1471	1496	rBV3	19690786	55615447	100.00%	51.288%
57	11.286	1537	1539	1545	rVB4	356	456	0.00%	0.000%
58	11.579	1585	1587	1588	rVV	247	216	0.00%	0.000%
59	11.627	1589	1595	1606	rVV	73013	128290	0.23%	0.118%
60	11.731	1606	1612	1617	rVB	8777	13898	0.02%	0.013%
61	11.835	1622	1629	1638	rVB	23016	39836	0.07%	0.037%
62	11.981	1650	1653	1657	rBV	512	787	0.00%	0.001%
63	12.121	1673	1676	1677	rBV2	208	193	0.00%	0.000%
64	12.164	1677	1683	1690	rVV	21336	34305	0.06%	0.032%
65	12.335	1707	1711	1712	rVV3	214	237	0.00%	0.000%
66	12.359	1712	1715	1719	rVB5	1366	2047	0.00%	0.002%
67	12.469	1730	1733	1736	rVB3	205	259	0.00%	0.000%
68	12.603	1750	1755	1761	rBV	7778	11643	0.02%	0.011%
69	12.694	1764	1770	1776	rVB	31797	52703	0.09%	0.049%
70	13.188	1850	1851	1854	rVB	494	315	0.00%	0.000%
71	13.243	1858	1860	1862	rBV2	233	317	0.00%	0.000%
72	13.273	1862	1865	1871	rVB4	548	1002	0.00%	0.001%
73	13.389	1882	1884	1885	rBV2	483	468	0.00%	0.000%
74	13.408	1885	1887	1889	rVB2	604	568	0.00%	0.001%
75	13.554	1905	1911	1917	rBV	32866	54783	0.10%	0.051%
76	13.853	1954	1960	1966	rVB	34151	53572	0.10%	0.049%

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Peak Location: TOP

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 Title : SFAM01.0

77	13.932	1971	1973	1979	rVB2	257	349	0.00%	0.000%
78	14.060	1990	1994	1998	rVB3	698	863	0.00%	0.001%
79	14.231	2018	2022	2024	rVB	272	390	0.00%	0.000%
80	14.261	2024	2027	2028	rBV	240	262	0.00%	0.000%
81	14.359	2040	2043	2047	rBV3	188	246	0.00%	0.000%
82	14.487	2060	2064	2067	rVB3	222	314	0.00%	0.000%
83	14.609	2082	2084	2087	rVB2	209	199	0.00%	0.000%
84	14.645	2087	2090	2092	rBV3	258	312	0.00%	0.000%
85	14.712	2096	2101	2102	rBV3	185	319	0.00%	0.000%
86	14.871	2126	2127	2131	rBV2	209	274	0.00%	0.000%
87	14.901	2131	2132	2134	rBV	247	203	0.00%	0.000%
88	14.962	2139	2142	2143	rBV2	291	321	0.00%	0.000%
89	15.358	2204	2207	2209	rBV2	202	276	0.00%	0.000%
90	15.432	2216	2219	2222	rVB3	357	506	0.00%	0.000%
91	15.486	2224	2228	2234	rVB4	346	650	0.00%	0.001%
92	15.681	2258	2260	2261	rVV	289	207	0.00%	0.000%
93	15.700	2261	2263	2265	rVB	371	336	0.00%	0.000%
94	15.730	2265	2268	2269	rBV2	290	363	0.00%	0.000%
95	16.157	2335	2338	2341	rVV2	241	326	0.00%	0.000%
96	16.230	2348	2350	2352	rVB2	262	189	0.00%	0.000%
97	16.334	2366	2367	2370	rBV	212	199	0.00%	0.000%
98	16.480	2388	2391	2394	rBV2	296	446	0.00%	0.000%
99	16.639	2415	2417	2420	rVB2	249	234	0.00%	0.000%
100	16.687	2422	2425	2427	rBV2	229	267	0.00%	0.000%

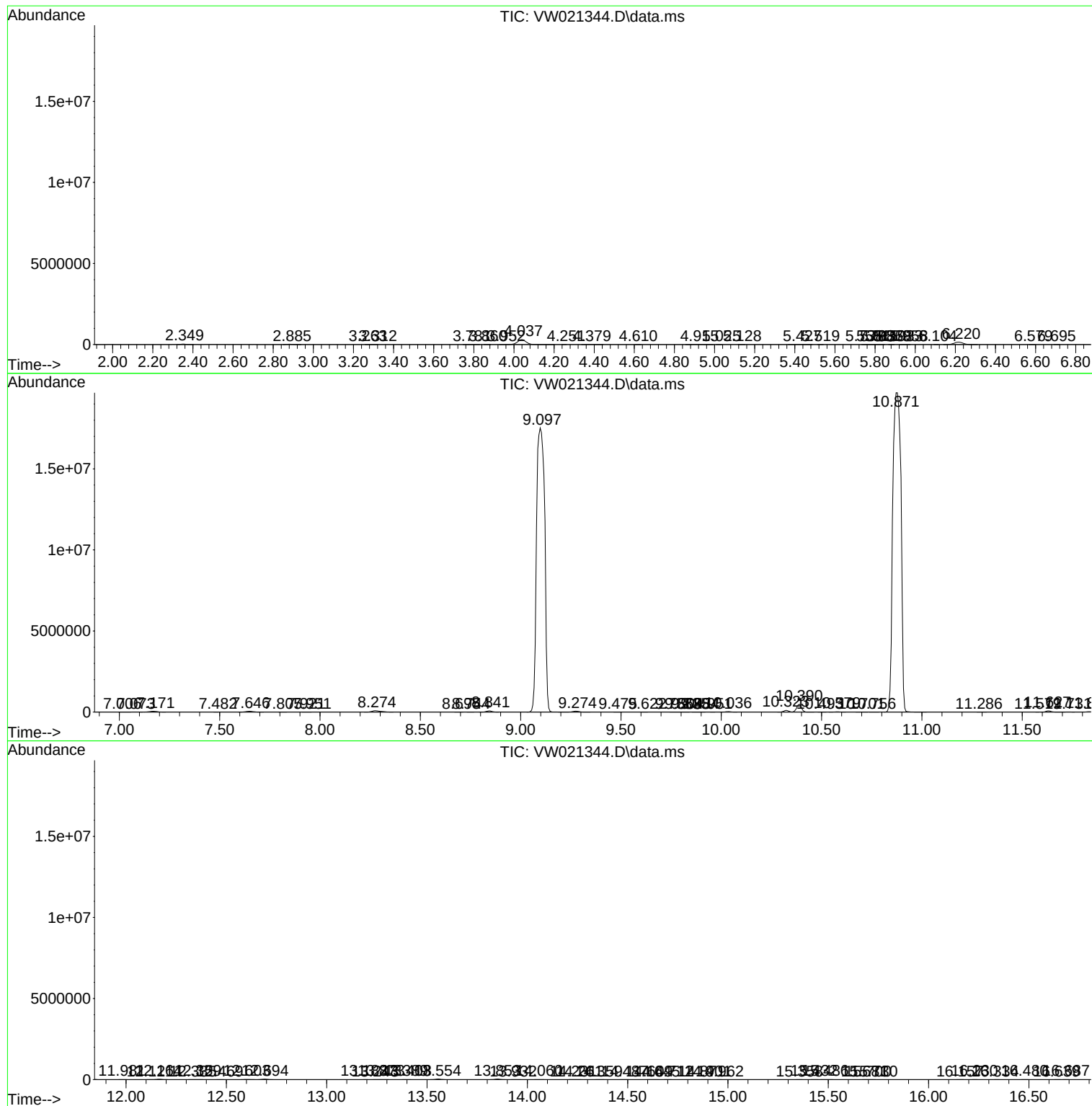
Sum of corrected areas: 108437721

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM120921SMA.M
Quant Title : SFAM01.0

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



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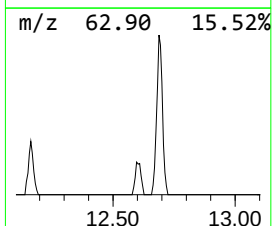
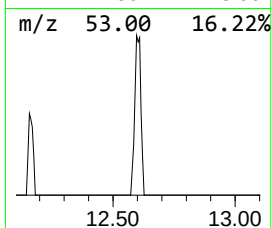
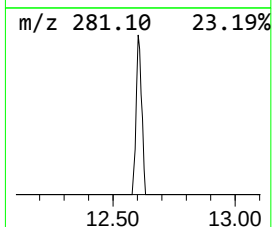
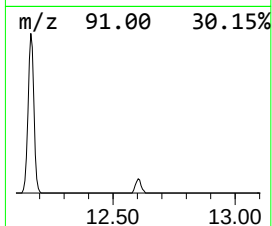
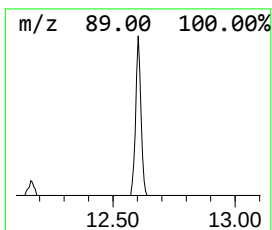
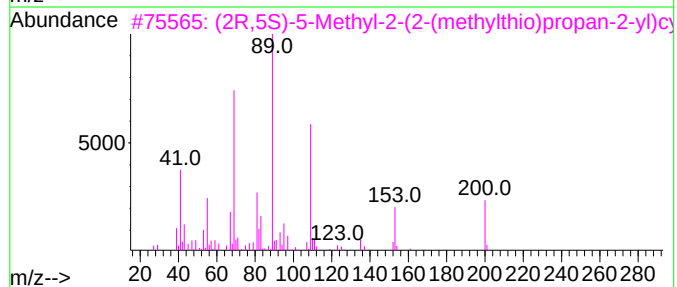
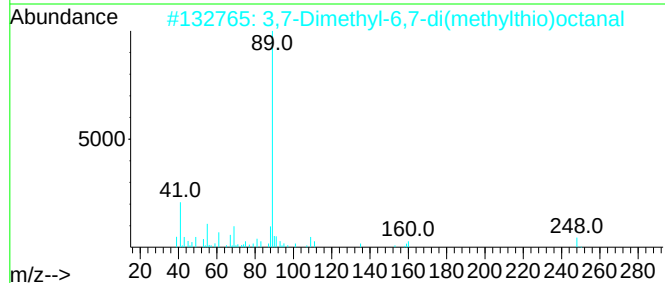
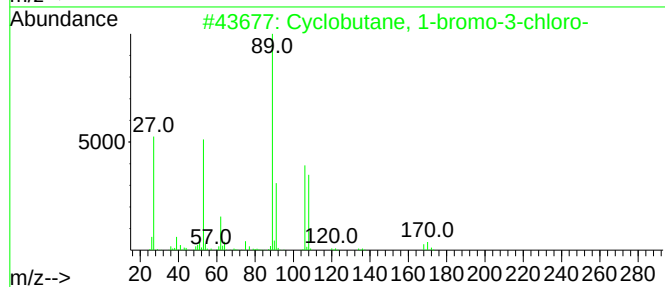
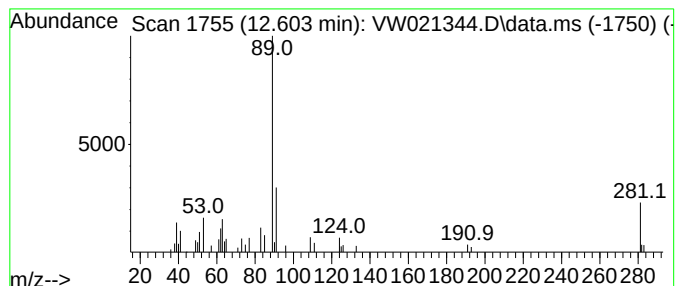
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM120921SMA.M
Quant Title : SFAM01.0

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

Peak Number 2 Cyclobutane, 1-bromo-3-chloro- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.603	5.31 ug/L	11643	1,4-Dichlorobenzene-d4	13.554

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclobutane, 1-bromo-3-chloro-	168	C4H6BrCl	004935-03-9	56
2			3,7-Dimethyl-6,7-di(methylthio)octanal	248	C12H24OS2	1000314-40-1	50
3			(2R,5S)-5-Methyl-2-(2-(methylthio)propan-2-yl)octanal	200	C11H20OS	032637-94-8	39
4			5-Ethyl-2,3,4,6-tetrathiaheptane	200	C5H12S4	126876-25-3	39
5			Diglycolic acid, 2-methoxyphenyl...	282	C14H18O6	1010382-24-0	38



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Cyclobutane, 1-...	12.603	5.3	ug/L	11643	3	13.554	54783	25.0