

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY120621\
 Data File : VY006972.D
 Acq On : 06 Dec 2021 19:31
 Operator : SY/MD
 Sample : M4887-20
 Misc : 5.47g/10.0mL/MSVOA_Y/SOIL
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 EX8D2

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_Y\methods\SFAMYL120321SMA.M
 Title : VOC Analysis

Signal : TIC: VY006972.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.247	64	70	83	rVB	40908	73085	18.59%	2.825%
2	2.765	149	155	167	rVB	22525	54210	13.79%	2.095%
3	3.247	233	234	237	rBV2	648	673	0.17%	0.026%
4	3.436	263	265	269	rBV2	261	217	0.06%	0.008%
5	3.558	282	285	290	rVB3	373	561	0.14%	0.022%
6	3.594	290	291	292	rBV	296	148	0.04%	0.006%
7	3.741	313	315	318	rBV	263	260	0.07%	0.010%
8	3.851	323	333	345	rBV	37717	116121	29.54%	4.489%
9	4.180	382	387	389	rBV2	1407	2282	0.58%	0.088%
10	4.283	401	404	408	rBV	281	319	0.08%	0.012%
11	4.369	415	418	419	rVB	174	143	0.04%	0.006%
12	4.539	444	446	448	rBV2	281	214	0.05%	0.008%
13	4.716	464	475	491	rVB2	10646	38163	9.71%	1.475%
14	4.893	503	504	509	rBV3	300	507	0.13%	0.020%
15	5.149	545	546	548	rVB	263	148	0.04%	0.006%
16	5.576	614	616	620	rVB	266	320	0.08%	0.012%
17	5.612	620	622	624	rBV	170	149	0.04%	0.006%
18	5.655	624	629	630	rVB	168	247	0.06%	0.010%
19	5.734	636	642	643	rBV3	1633	2304	0.59%	0.089%
20	5.911	669	671	675	rVB	290	274	0.07%	0.011%
21	6.009	682	687	689	rBV2	205	347	0.09%	0.013%
22	6.167	711	713	717	rVB2	151	204	0.05%	0.008%
23	6.210	717	720	725	rBV2	301	597	0.15%	0.023%
24	6.332	739	740	743	rVB2	418	383	0.10%	0.015%
25	6.362	743	745	746	rBV	198	187	0.05%	0.007%
26	6.442	755	758	760	rBV2	144	186	0.05%	0.007%
27	6.478	762	764	768	rVB2	242	299	0.08%	0.012%
28	6.515	768	770	771	rBV	286	241	0.06%	0.009%
29	6.789	813	815	817	rBV	387	402	0.10%	0.016%
30	6.880	820	830	831	rBV	9947	16264	4.14%	0.629%
31	7.191	880	881	883	rBV2	346	310	0.08%	0.012%
32	7.319	901	902	906	rBV3	390	474	0.12%	0.018%
33	7.478	918	928	941	rVB	63711	161203	41.00%	6.231%
34	7.673	959	960	964	rVB	307	181	0.05%	0.007%
35	7.710	964	966	969	rBV	218	293	0.07%	0.011%
36	7.892	994	996	999	rBV2	239	399	0.10%	0.015%

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Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\SFAMYL120321SMA.M
 Title : VOC Analysis

37	8.112	1022	1032	1047	rVB3	129502	393151	100.00%	15.197%
38	8.234	1047	1052	1056	rBV3	1109	1663	0.42%	0.064%
39	8.289	1059	1061	1062	rBV	273	238	0.06%	0.009%
40	8.374	1072	1075	1076	rBV2	176	203	0.05%	0.008%
41	8.478	1090	1092	1093	rVB	544	282	0.07%	0.011%
42	8.496	1093	1095	1099	rBV2	293	425	0.11%	0.016%
43	8.533	1099	1101	1103	rBV	435	351	0.09%	0.014%
44	8.587	1108	1110	1113	rVV2	179	160	0.04%	0.006%
45	8.685	1118	1126	1137	rVB	137942	269908	68.65%	10.433%
46	8.935	1161	1167	1172	rVB7	3490	6543	1.66%	0.253%
47	9.118	1186	1197	1206	rVV	88755	178265	45.34%	6.891%
48	9.252	1217	1219	1220	rBV2	283	179	0.05%	0.007%
49	9.362	1235	1237	1238	rBV	256	222	0.06%	0.009%
50	9.490	1255	1258	1261	rBV	237	321	0.08%	0.012%
51	9.526	1261	1264	1267	rBV	201	297	0.08%	0.011%
52	9.642	1282	1283	1288	rBV2	211	229	0.06%	0.009%
53	9.685	1288	1290	1293	rVB	309	304	0.08%	0.012%
54	9.782	1304	1306	1309	rVB3	372	399	0.10%	0.015%
55	9.819	1309	1312	1313	rBV	236	179	0.05%	0.007%
56	9.886	1317	1323	1336	rVB	44952	77376	19.68%	2.991%
57	9.990	1336	1340	1344	rVB2	250	353	0.09%	0.014%
58	10.069	1346	1353	1356	rBV5	1058	2082	0.53%	0.080%
59	10.179	1364	1371	1378	rBV	159581	270138	68.71%	10.442%
60	10.240	1378	1381	1388	rVB2	3067	4727	1.20%	0.183%
61	10.343	1396	1398	1399	rVB2	325	163	0.04%	0.006%
62	10.435	1406	1413	1421	rVB2	27070	47500	12.08%	1.836%
63	10.575	1430	1436	1443	rVB2	11546	20810	5.29%	0.804%
64	10.715	1455	1459	1464	rVB3	3352	5171	1.32%	0.200%
65	10.788	1464	1471	1484	rBV3	35605	80002	20.35%	3.092%
66	10.947	1490	1497	1503	rBV	16085	29003	7.38%	1.121%
67	11.264	1546	1549	1551	rBV	469	469	0.12%	0.018%
68	11.313	1551	1557	1564	rVV2	9337	15970	4.06%	0.617%
69	11.361	1564	1565	1568	rBV	241	229	0.06%	0.009%
70	11.489	1578	1586	1597	rVB	151803	249602	63.49%	9.648%
71	11.569	1597	1599	1601	rBV2	297	349	0.09%	0.013%
72	11.593	1601	1603	1605	rBV2	318	226	0.06%	0.009%
73	11.636	1608	1610	1613	rBV2	219	194	0.05%	0.007%
74	11.691	1617	1619	1620	rBV	359	261	0.07%	0.010%
75	11.764	1629	1631	1635	rBV	162	206	0.05%	0.008%
76	11.928	1657	1658	1662	rBV	298	300	0.08%	0.012%

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77	12.093	1684	1685	1687	rVB	357	193	0.05%	0.007%
78	12.178	1697	1699	1701	rBV3	235	185	0.05%	0.007%
79	12.258	1710	1712	1713	rVB2	273	146	0.04%	0.006%
80	12.318	1721	1722	1724	rBV2	378	200	0.05%	0.008%
81	12.379	1729	1732	1733	rVB	184	153	0.04%	0.006%
82	12.489	1739	1750	1756	rBV	38913	65605	16.69%	2.536%
83	12.556	1756	1761	1769	rVB	54756	88059	22.40%	3.404%
84	12.623	1769	1772	1774	rBV3	514	671	0.17%	0.026%
85	12.678	1780	1781	1784	rBV2	263	261	0.07%	0.010%
86	12.764	1790	1795	1800	rBV	3965	6821	1.73%	0.264%
87	12.818	1800	1804	1810	rVB2	6049	9324	2.37%	0.360%
88	13.062	1840	1844	1849	rBV3	1454	2449	0.62%	0.095%
89	13.178	1860	1863	1868	rVB2	2687	3851	0.98%	0.149%
90	13.276	1874	1879	1885	rVB5	1012	1854	0.47%	0.072%
91	13.343	1889	1890	1894	rBV3	321	239	0.06%	0.009%
92	13.422	1897	1903	1909	rVV	101300	151296	38.48%	5.848%
93	13.477	1909	1912	1916	rVV5	1573	2751	0.70%	0.106%
94	13.526	1916	1920	1926	rVB4	3221	5621	1.43%	0.217%
95	13.629	1935	1937	1939	rBV2	756	725	0.18%	0.028%
96	13.721	1945	1952	1960	rBV	62937	100694	25.61%	3.892%
97	13.958	1987	1991	2001	rVB2	7807	12729	3.24%	0.492%
98	14.056	2005	2007	2009	rBV2	482	532	0.14%	0.021%
99	14.885	2141	2143	2148	rBV2	711	1079	0.27%	0.042%
100	15.147	2184	2186	2188	rBV2	1005	869	0.22%	0.034%

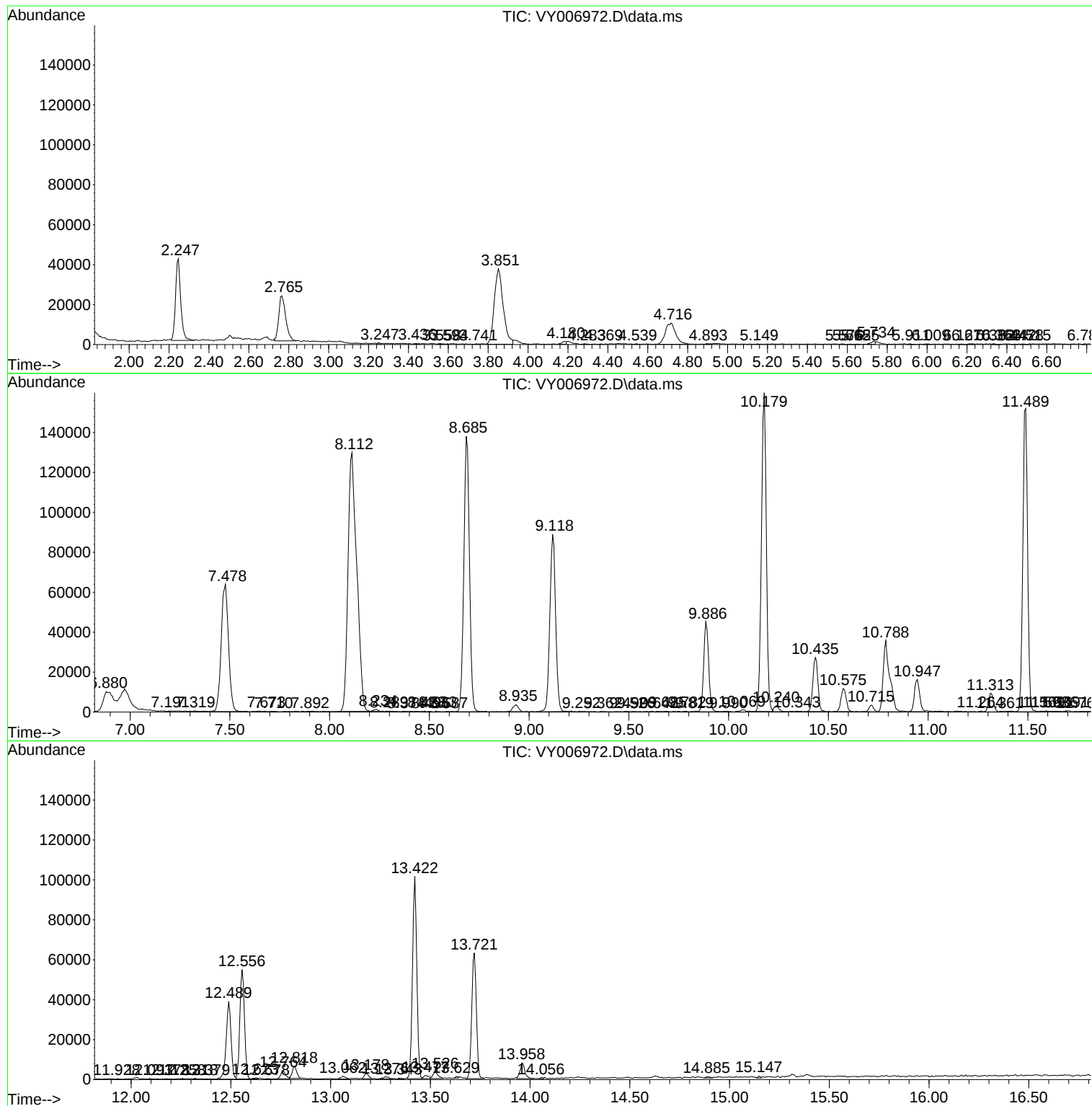
Sum of corrected areas: 2587072

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\SFAMLYM120321SMA.M
Quant Title : VOC Analysis

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



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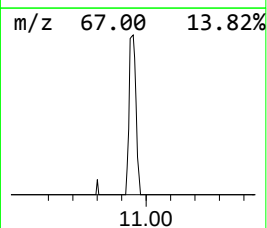
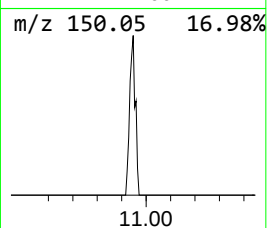
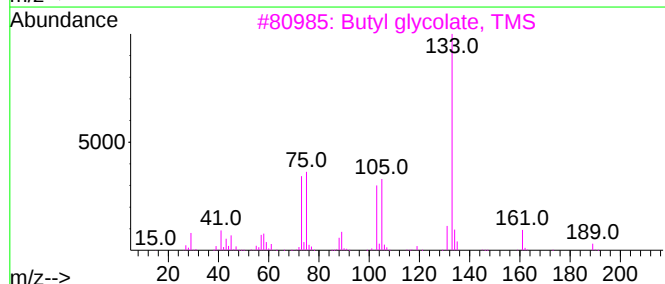
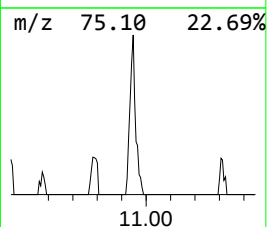
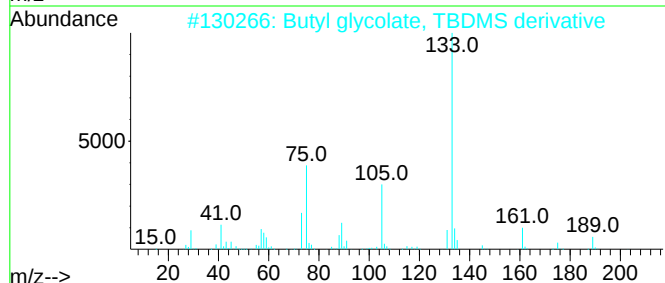
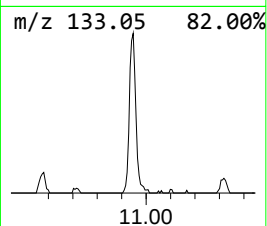
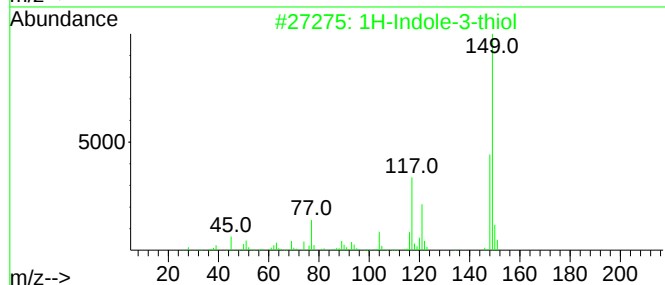
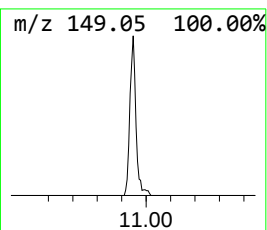
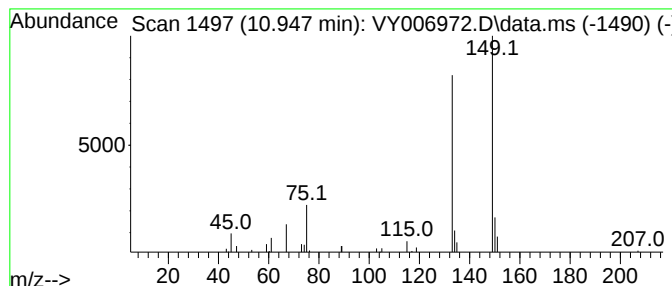
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\SFAMYL120321SMA.M
Quant Title : VOC Analysis

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

Peak Number 4 unknown-01 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.947	2.90 ug/L	29003	Chlorobenzene-d5	11.489

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Indole-3-thiol	149	C8H7NS	000480-94-4	35
2			Butyl glycolate, TBDMS derivative	246	C12H26O3Si	1000366-87-5	32
3			Butyl glycolate, TMS	204	C9H20O3Si	087826-84-4	25
4			Butyl glycolate, (3-cyanopropyl)...	257	C12H23NO3Si	1010376-00-0	23
5			(1-t-Butylthiovinyl)oxy)trimethyl...	204	C9H20O5Si	063584-47-4	23



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	10.947	2.9	ug/L	29003	2	11.489	249602	25.0