

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY120421\
 Data File : VY006943.D
 Acq On : 04 Dec 2021 15:48
 Operator : SY/MD
 Sample : M4884-13
 Misc : 3.54g/10.0mL/MSVOA_Y/SOIL
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 EW9J9

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: VY006943.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	79	rVB	56735	94771	1.78%	1.008%
2	2.510	109	113	120	rBV6	1626	4152	0.08%	0.044%
3	2.766	147	155	170	rBV	32819	81484	1.53%	0.867%
4	2.900	175	177	181	rBV3	703	851	0.02%	0.009%
5	3.028	196	198	200	rBV2	565	334	0.01%	0.004%
6	3.156	218	219	222	rVB	541	399	0.01%	0.004%
7	3.186	222	224	228	rBV	223	321	0.01%	0.003%
8	3.643	297	299	302	rVB2	330	326	0.01%	0.003%
9	3.851	323	333	348	rBV2	65042	184798	3.48%	1.966%
10	4.198	382	390	399	rVV2	2393	7029	0.13%	0.075%
11	4.320	407	410	413	rVB	319	381	0.01%	0.004%
12	4.540	444	446	450	rBV2	320	500	0.01%	0.005%
13	4.716	464	475	489	rBV3	9800	32451	0.61%	0.345%
14	4.899	502	505	507	rBV	312	308	0.01%	0.003%
15	4.942	509	512	515	rVV3	412	430	0.01%	0.005%
16	5.046	526	529	533	rBV2	297	507	0.01%	0.005%
17	5.125	539	542	544	rBV	246	343	0.01%	0.004%
18	5.747	635	644	654	rBV4	2139	6353	0.12%	0.068%
19	6.582	779	781	784	rBV2	263	320	0.01%	0.003%
20	6.783	810	814	816	rBV3	406	507	0.01%	0.005%
21	6.887	820	831	840	rBV	28141	83710	1.58%	0.891%
22	6.984	841	847	859	rVB2	8719	27713	0.52%	0.295%
23	7.478	918	928	944	rVV	97281	248149	4.67%	2.640%
24	7.673	957	960	961	rBV2	340	354	0.01%	0.004%
25	7.692	961	963	965	rVV3	463	345	0.01%	0.004%
26	8.015	1012	1016	1018	rVV3	287	406	0.01%	0.004%
27	8.112	1021	1032	1046	rVV2	198279	602668	11.34%	6.411%
28	8.234	1047	1052	1060	rVB2	4869	9242	0.17%	0.098%
29	8.691	1118	1127	1135	rBV	170028	329552	6.20%	3.506%
30	8.941	1158	1168	1181	rVV	2836643	5312266	100.00%	56.512%
31	9.124	1188	1198	1206	rBV	131130	270298	5.09%	2.875%
32	9.356	1233	1236	1237	rBV2	484	638	0.01%	0.007%
33	9.563	1266	1270	1271	rVB3	296	355	0.01%	0.004%
34	9.618	1276	1279	1282	rVB2	274	351	0.01%	0.004%
35	9.722	1294	1296	1301	rBV3	243	347	0.01%	0.004%
36	9.892	1316	1324	1331	rVB	68796	123265	2.32%	1.311%

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37	9.953	1331	1334	1338	rVB3	349	482	0.01%	0.005%
38	10.051	1348	1350	1351	rBV	501	467	0.01%	0.005%
39	10.063	1351	1352	1357	rVB3	930	1181	0.02%	0.013%
40	10.179	1363	1371	1378	rBV	212899	361009	6.80%	3.840%
41	10.246	1378	1382	1387	rVB	6294	9741	0.18%	0.104%
42	10.386	1399	1405	1407	rBV2	228	319	0.01%	0.003%
43	10.435	1407	1413	1421	rVB	42758	71519	1.35%	0.761%
44	10.575	1429	1436	1442	rBV2	26561	48224	0.91%	0.513%
45	10.642	1442	1447	1454	rVB	55962	95669	1.80%	1.018%
46	10.715	1454	1459	1465	rVB3	11862	20458	0.39%	0.218%
47	10.789	1465	1471	1482	rBV	87320	144961	2.73%	1.542%
48	10.947	1490	1497	1503	rBV2	15044	27703	0.52%	0.295%
49	11.038	1509	1512	1513	rBV2	623	505	0.01%	0.005%
50	11.087	1517	1520	1524	rBV3	416	505	0.01%	0.005%
51	11.313	1549	1557	1567	rVB2	23832	41225	0.78%	0.439%
52	11.392	1567	1570	1575	rBV2	289	455	0.01%	0.005%
53	11.490	1578	1586	1596	rBV	175982	288949	5.44%	3.074%
54	11.587	1601	1602	1605	rVV	302	325	0.01%	0.003%
55	11.697	1614	1620	1624	rVB4	1125	1661	0.03%	0.018%
56	11.831	1636	1642	1643	rBV2	249	426	0.01%	0.005%
57	11.935	1656	1659	1660	rVV2	414	293	0.01%	0.003%
58	12.020	1671	1673	1680	rVB3	963	1376	0.03%	0.015%
59	12.203	1699	1703	1706	rBV	204	361	0.01%	0.004%
60	12.331	1721	1724	1728	rVB2	1168	1277	0.02%	0.014%
61	12.489	1741	1750	1756	rBV	116538	192165	3.62%	2.044%
62	12.557	1756	1761	1768	rVV	96608	154259	2.90%	1.641%
63	12.624	1768	1772	1775	rVV2	633	827	0.02%	0.009%
64	12.666	1776	1779	1780	rVB2	384	306	0.01%	0.003%
65	12.733	1787	1790	1791	rBV2	319	309	0.01%	0.003%
66	12.758	1792	1794	1799	rVV4	854	1368	0.03%	0.015%
67	12.819	1799	1804	1813	rVV2	5665	9879	0.19%	0.105%
68	12.898	1815	1817	1822	rVB2	514	699	0.01%	0.007%
69	12.953	1825	1826	1828	rVV	559	304	0.01%	0.003%
70	13.038	1837	1840	1841	rVV2	323	290	0.01%	0.003%
71	13.069	1841	1845	1849	rVB4	1891	2976	0.06%	0.032%
72	13.117	1851	1853	1856	rVV2	613	577	0.01%	0.006%
73	13.184	1858	1864	1869	rVB	11232	17605	0.33%	0.187%
74	13.282	1873	1880	1884	rBV5	2686	4883	0.09%	0.052%
75	13.361	1891	1893	1894	rVV2	625	577	0.01%	0.006%
76	13.422	1896	1903	1909	rVV	121688	191381	3.60%	2.036%

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77	13.483	1909	1913	1917	rVV6	3242	6352	0.12%	0.068%
78	13.526	1918	1920	1928	rVB4	1981	2853	0.05%	0.030%
79	13.642	1933	1939	1945	rBV4	1890	4227	0.08%	0.045%
80	13.721	1945	1952	1960	rBV	124273	196326	3.70%	2.089%
81	13.825	1967	1969	1971	rBV2	585	387	0.01%	0.004%
82	13.965	1986	1992	2000	rVB2	25574	44655	0.84%	0.475%
83	14.032	2000	2003	2004	rBV2	414	499	0.01%	0.005%
84	14.081	2009	2011	2015	rVB3	541	728	0.01%	0.008%
85	14.178	2025	2027	2028	rVV2	525	327	0.01%	0.003%
86	14.233	2034	2036	2037	rBV2	437	318	0.01%	0.003%
87	14.276	2041	2043	2045	rVB3	602	395	0.01%	0.004%
88	14.343	2052	2054	2055	rVB2	563	341	0.01%	0.004%
89	14.629	2094	2101	2105	rVB6	2071	4033	0.08%	0.043%
90	14.727	2114	2117	2119	rBV4	516	606	0.01%	0.006%
91	14.751	2119	2121	2122	rBV2	472	397	0.01%	0.004%
92	14.855	2136	2138	2141	rBV	414	341	0.01%	0.004%
93	15.111	2176	2180	2183	rVB5	867	1265	0.02%	0.013%
94	15.190	2191	2193	2196	rBV4	514	540	0.01%	0.006%
95	15.233	2198	2200	2204	rVB5	1454	1579	0.03%	0.017%
96	15.318	2209	2214	2218	rVV4	3037	5350	0.10%	0.057%
97	15.385	2222	2225	2230	rVB3	2234	3015	0.06%	0.032%
98	15.751	2283	2285	2288	rVB4	897	738	0.01%	0.008%
99	16.714	2441	2443	2445	rBV3	731	501	0.01%	0.005%
100	16.781	2452	2454	2455	rBV2	834	709	0.01%	0.008%

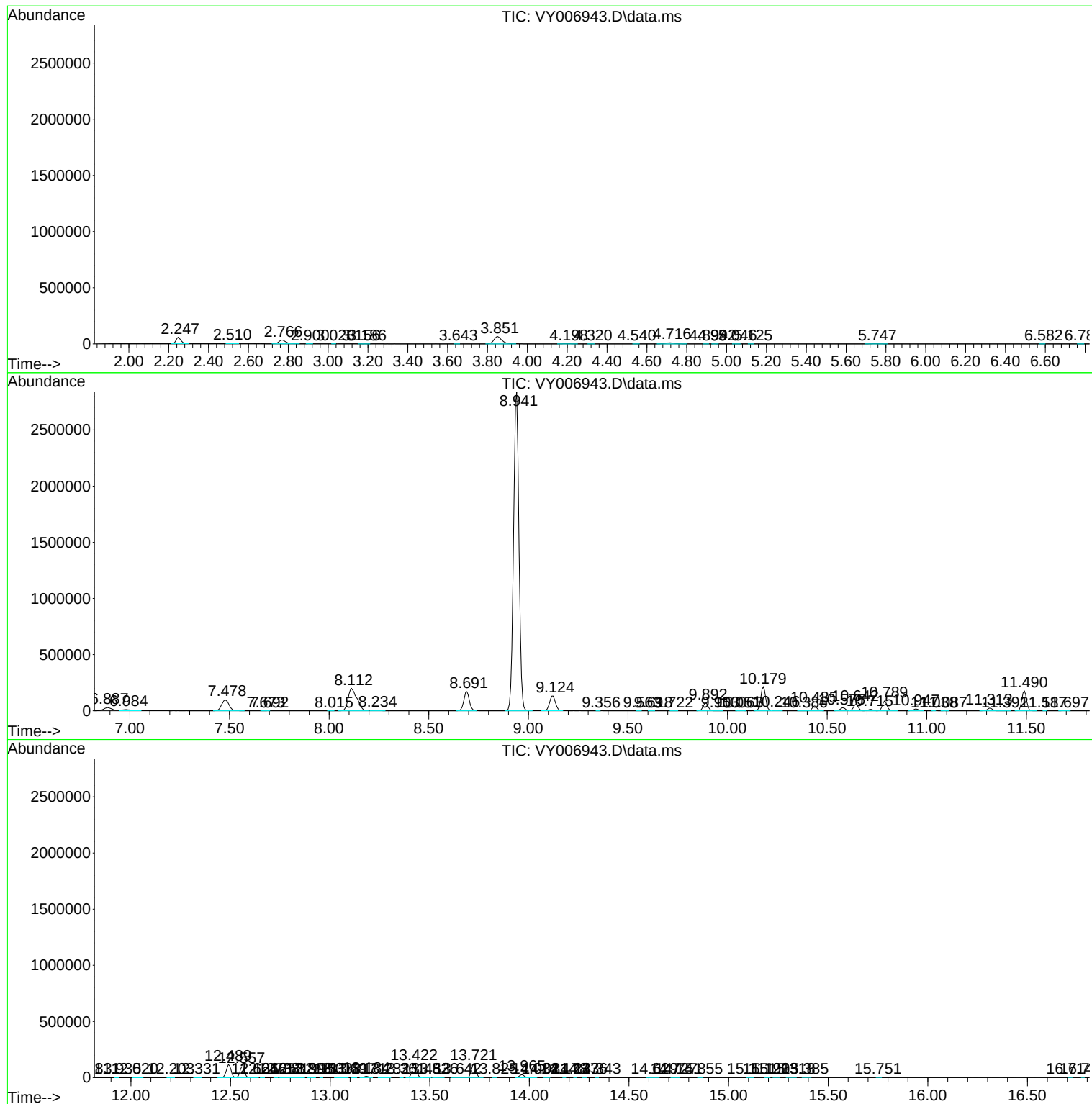
Sum of corrected areas: 9400202

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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



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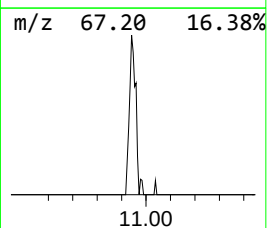
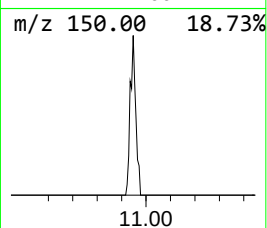
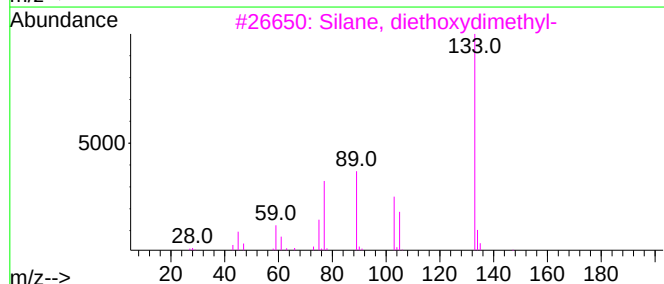
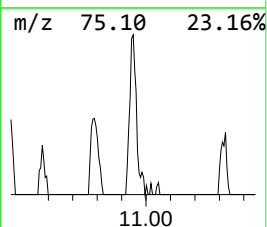
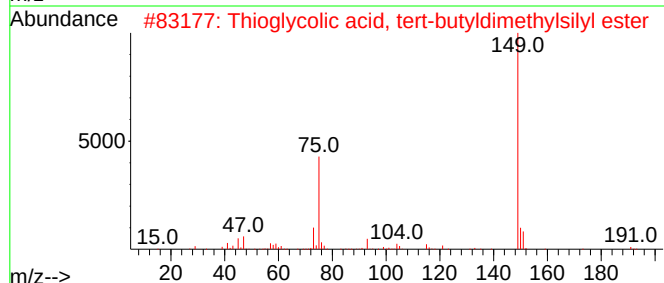
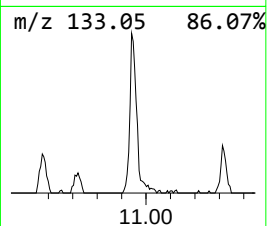
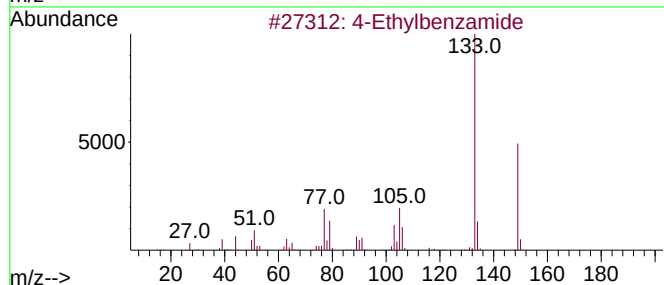
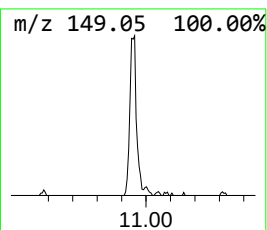
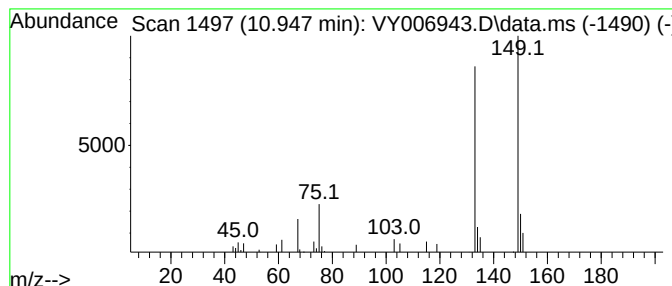
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\SFAMYL120321SMA.M
Quant Title : VOC Analysis

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

Peak Number 5 unknown-01 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.947	2.40 ug/L	27703	Chlorobenzene-d5	11.490

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Ethylbenzamide	149	C9H11NO	033695-58-8	45
2			Thioglycolic acid, tert-butyldim...	206	C8H18O2SSi	1000476-01-2	43
3			Silane, diethoxydimethyl-	148	C6H16O2Si	000078-62-6	27
4			1,2,4-Triazole, 3,5-dithioxo-	133	C2H3N3S2	005650-03-3	27
5			Silane, diethoxymethyloctadecyl-	386	C23H50O2Si	067859-75-0	27



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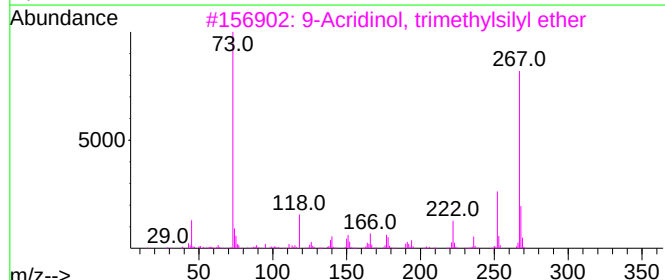
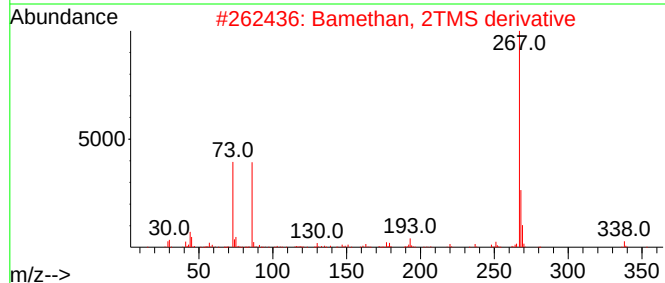
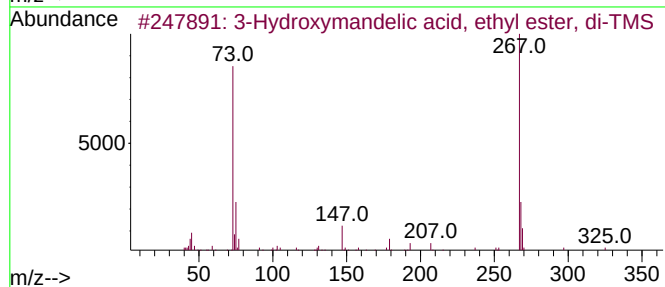
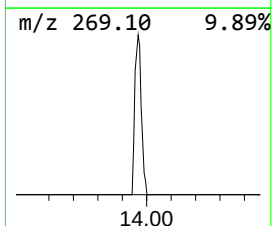
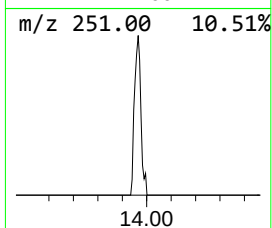
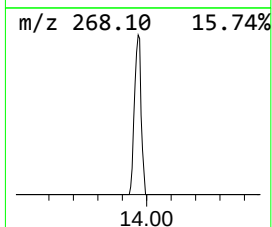
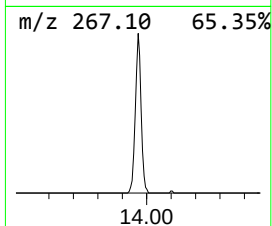
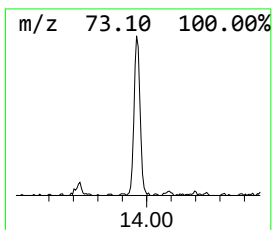
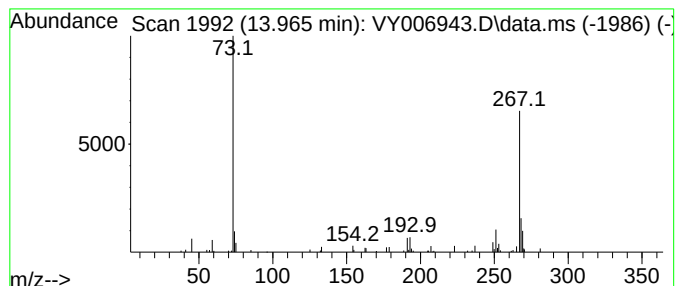
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Quant Title : VOC Analysis

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

Peak Number 10 Bamethan, 2TMS derivative Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.965	5.83 ug/L	44655	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Hydroxymandelic acid, ethyl es...	340	C16H28O4Si2	1000071-88-9	64
2			Bamethan, 2TMS derivative	353	C18H35NO2Si2	040629-66-1	64
3			9-Acridinol, trimethylsilyl ether	267	C16H17NOSi	1000463-65-5	59
4			Benzeneethanamine, N-[(pentaflu...	475	C21H26F5NO2Si2	055429-85-1	59
5			Salicylic acid, 2TMS derivative	282	C13H22O3Si2	003789-85-3	59



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	10.947	2.4	ug/L	27703	2	11.490	288949	25.0
Bamethan, 2TMS ...	13.965	5.8	ug/L	44655	3	13.422	191381	25.0