

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY120421\
 Data File : VY006931.D
 Acq On : 04 Dec 2021 11:24
 Operator : SY/MD
 Sample : M4884-01
 Misc : 2.32g/10.0mL/MSVOA_Y/SOIL
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 EW9H7

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: VY006931.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.253	66	71	78	rVB	24133	40550	9.86%	1.315%
2	2.772	150	156	168	rVB	17479	41718	10.15%	1.353%
3	3.241	231	233	236	rBV3	308	362	0.09%	0.012%
4	3.357	251	252	254	rBV	262	191	0.05%	0.006%
5	3.387	254	257	263	rVB2	541	723	0.18%	0.023%
6	3.497	273	275	276	rBV	258	212	0.05%	0.007%
7	3.601	290	292	293	rVB	300	211	0.05%	0.007%
8	3.686	298	306	310	rBV2	219	630	0.15%	0.020%
9	3.747	313	316	318	rBV3	349	460	0.11%	0.015%
10	3.851	323	333	345	rBV2	38699	108104	26.30%	3.507%
11	4.198	380	390	401	rBV3	2416	8236	2.00%	0.267%
12	4.326	407	411	414	rBB2	155	283	0.07%	0.009%
13	4.418	424	426	429	rVV2	171	211	0.05%	0.007%
14	4.479	435	436	439	rBV	213	217	0.05%	0.007%
15	4.649	461	464	466	rBV	247	298	0.07%	0.010%
16	4.722	466	476	490	rVB3	13904	43313	10.54%	1.405%
17	4.893	502	504	505	rBV3	339	261	0.06%	0.008%
18	4.911	505	507	509	rVV2	443	362	0.09%	0.012%
19	5.021	522	525	526	rBV	192	201	0.05%	0.007%
20	5.210	554	556	558	rVB	292	201	0.05%	0.007%
21	5.417	587	590	593	rVB	179	238	0.06%	0.008%
22	5.503	600	604	607	rVB2	275	412	0.10%	0.013%
23	5.619	620	623	626	rBV	203	267	0.06%	0.009%
24	5.740	638	643	652	rVB4	1985	5560	1.35%	0.180%
25	5.923	670	673	674	rBV	233	200	0.05%	0.006%
26	5.997	683	685	688	rVB2	250	236	0.06%	0.008%
27	6.070	694	697	698	rBV2	186	224	0.05%	0.007%
28	6.216	719	721	725	rBV	222	266	0.06%	0.009%
29	6.289	729	733	735	rBV	278	348	0.08%	0.011%
30	6.442	755	758	760	rBV	240	302	0.07%	0.010%
31	6.551	774	776	779	rBV2	124	188	0.05%	0.006%
32	6.625	786	788	792	rVB	216	219	0.05%	0.007%
33	6.887	823	831	840	rBV	15134	41982	10.21%	1.362%
34	6.984	843	847	858	rVB	5149	14328	3.49%	0.465%
35	7.307	896	900	902	rBV	183	335	0.08%	0.011%
36	7.478	919	928	942	rVB	58589	147143	35.80%	4.773%

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37	7.588	942	946	952	rVB2	287	548	0.13%	0.018%
38	7.643	952	955	958	rBV	242	283	0.07%	0.009%
39	7.691	960	963	965	rBV	269	294	0.07%	0.010%
40	7.819	982	984	987	rBV	202	200	0.05%	0.006%
41	8.118	1024	1033	1046	rVV2	115808	353583	86.02%	11.470%
42	8.240	1047	1053	1061	rVB4	3553	7661	1.86%	0.249%
43	8.362	1072	1073	1076	rVB2	319	298	0.07%	0.010%
44	8.405	1076	1080	1081	rBV2	171	255	0.06%	0.008%
45	8.453	1084	1088	1091	rBV	179	310	0.08%	0.010%
46	8.691	1117	1127	1137	rBV	209793	411064	100.00%	13.334%
47	8.783	1141	1142	1146	rBV	219	248	0.06%	0.008%
48	8.844	1150	1152	1156	rVV2	246	269	0.07%	0.009%
49	8.880	1156	1158	1162	rVV2	215	298	0.07%	0.010%
50	8.935	1162	1167	1173	rVB5	1160	2225	0.54%	0.072%
51	9.014	1178	1180	1183	rVB5	216	186	0.05%	0.006%
52	9.045	1183	1185	1187	rBV	267	300	0.07%	0.010%
53	9.124	1187	1198	1207	rBV	79644	157313	38.27%	5.103%
54	9.270	1220	1222	1225	rVB	322	278	0.07%	0.009%
55	9.490	1254	1258	1259	rBV2	262	286	0.07%	0.009%
56	9.514	1259	1262	1265	rVB3	541	757	0.18%	0.025%
57	9.648	1282	1284	1285	rBV	254	218	0.05%	0.007%
58	9.752	1296	1301	1304	rBV	423	629	0.15%	0.020%
59	9.837	1309	1315	1317	rBV	355	562	0.14%	0.018%
60	9.892	1317	1324	1332	rVB	42868	76518	18.61%	2.482%
61	9.959	1332	1335	1336	rBV	203	247	0.06%	0.008%
62	10.069	1349	1353	1357	rBV2	945	1576	0.38%	0.051%
63	10.185	1364	1372	1378	rBV	134029	232469	56.55%	7.541%
64	10.246	1378	1382	1389	rVB	9846	17354	4.22%	0.563%
65	10.337	1395	1397	1401	rVB2	235	288	0.07%	0.009%
66	10.374	1401	1403	1407	rBV2	309	389	0.09%	0.013%
67	10.441	1407	1414	1422	rBV	26983	45296	11.02%	1.469%
68	10.581	1430	1437	1444	rBV	30857	52870	12.86%	1.715%
69	10.715	1454	1459	1462	rBV3	557	977	0.24%	0.032%
70	10.788	1464	1471	1481	rBV	47343	80064	19.48%	2.597%
71	10.904	1487	1490	1492	rBV2	530	698	0.17%	0.023%
72	10.947	1492	1497	1507	rVV	17299	30882	7.51%	1.002%
73	11.038	1509	1512	1517	rVB5	1014	1861	0.45%	0.060%
74	11.179	1532	1535	1536	rVB	358	304	0.07%	0.010%
75	11.209	1536	1540	1542	rBV2	407	535	0.13%	0.017%
76	11.240	1542	1545	1547	rBV2	305	349	0.08%	0.011%

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77	11.319	1552	1558	1567	rVB	23506	39341	9.57%	1.276%
78	11.435	1575	1577	1579	rBV	314	371	0.09%	0.012%
79	11.489	1579	1586	1598	rVV	237850	391129	95.15%	12.688%
80	11.599	1598	1604	1609	rVV2	1736	3093	0.75%	0.100%
81	11.697	1616	1620	1626	rBV2	5611	9941	2.42%	0.322%
82	11.843	1642	1644	1647	rBV3	275	305	0.07%	0.010%
83	12.032	1670	1675	1682	rVB4	3780	6741	1.64%	0.219%
84	12.288	1715	1717	1719	rBV	210	206	0.05%	0.007%
85	12.331	1720	1724	1734	rVB5	1739	3018	0.73%	0.098%
86	12.495	1742	1751	1757	rBV	126107	206535	50.24%	6.700%
87	12.562	1757	1762	1768	rVB	57377	91241	22.20%	2.960%
88	12.733	1788	1790	1792	rBV2	354	314	0.08%	0.010%
89	12.825	1800	1805	1810	rBV3	7677	12172	2.96%	0.395%
90	12.965	1824	1828	1832	rVB5	683	954	0.23%	0.031%
91	13.075	1841	1846	1851	rVB3	1309	2082	0.51%	0.068%
92	13.123	1851	1854	1859	rBV2	1772	2384	0.58%	0.077%
93	13.184	1859	1864	1869	rVB2	11078	16209	3.94%	0.526%
94	13.282	1874	1880	1884	rBV4	2137	3433	0.84%	0.111%
95	13.428	1898	1904	1910	rBV	126762	189839	46.18%	6.158%
96	13.727	1947	1953	1960	rBV	74912	119981	29.19%	3.892%
97	13.965	1987	1992	2000	rVB2	22364	38498	9.37%	1.249%
98	14.074	2009	2010	2011	rBV	640	355	0.09%	0.012%
99	15.007	2160	2163	2164	rBV3	1687	1628	0.40%	0.053%
100	15.239	2198	2201	2206	rBV3	2299	3231	0.79%	0.105%

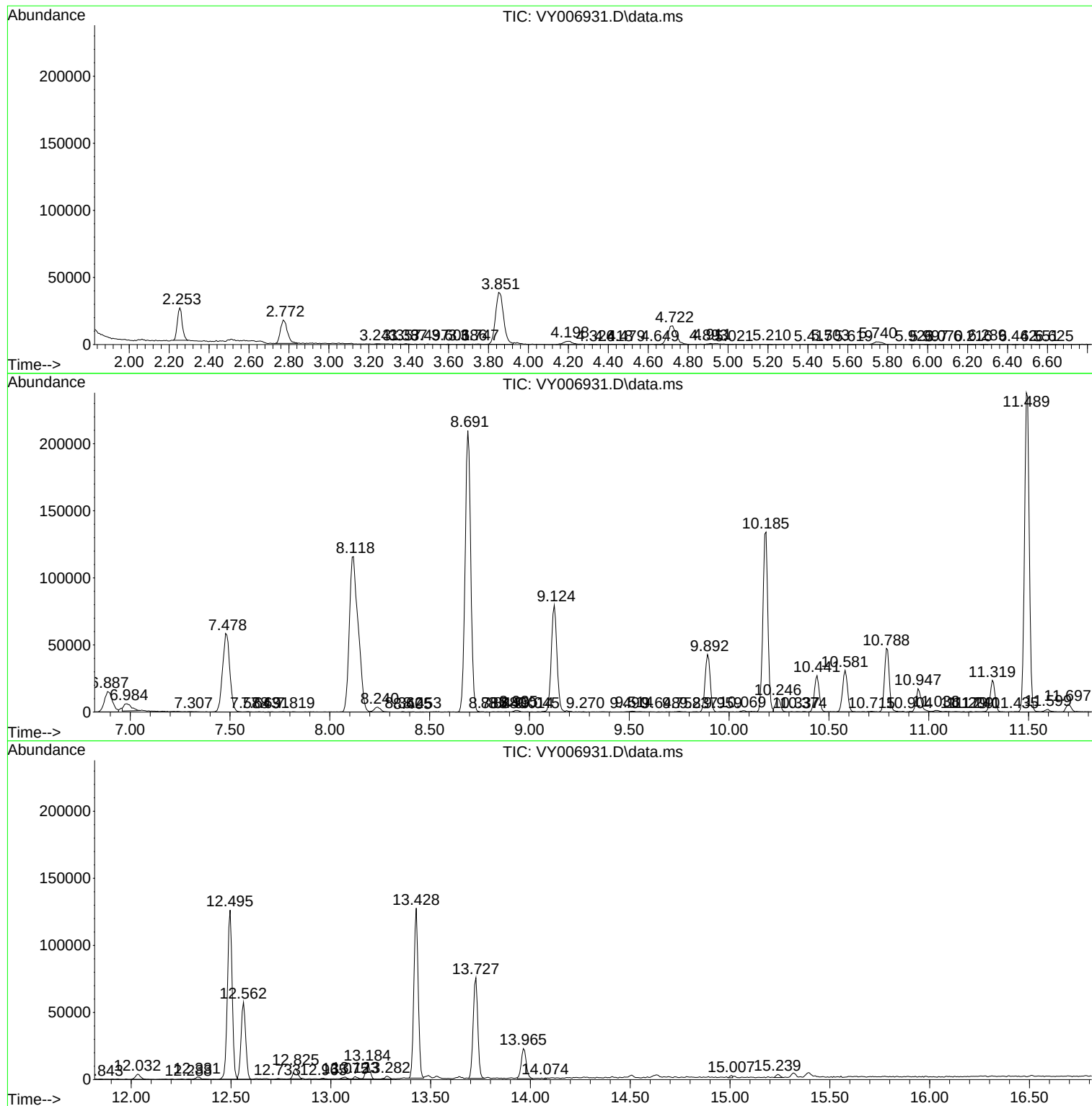
Sum of corrected areas: 3082735

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\SFAMYL120321SMA.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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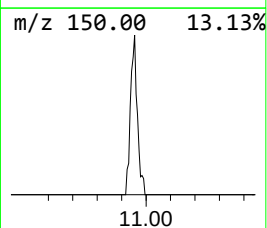
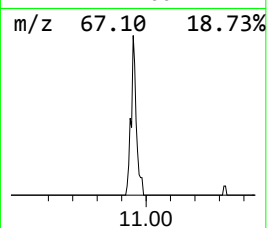
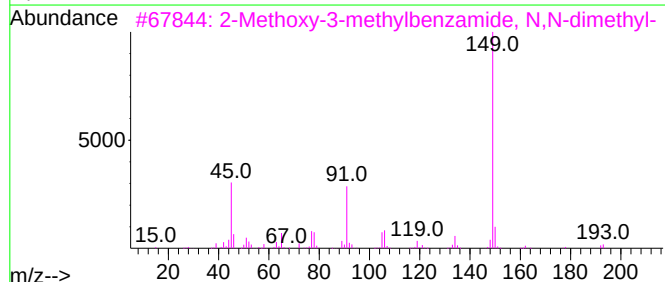
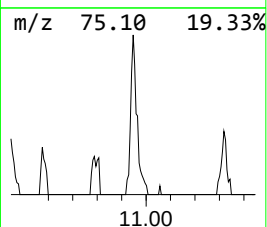
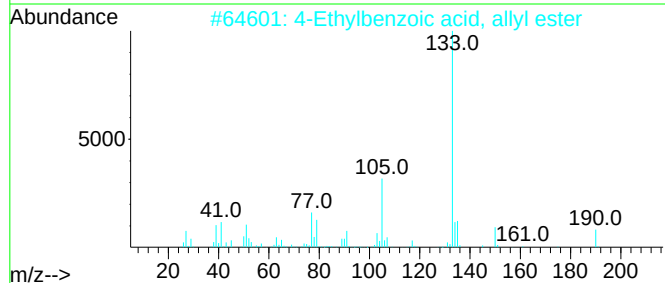
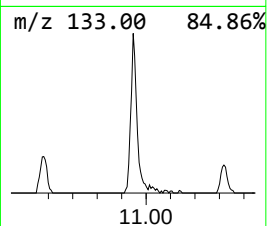
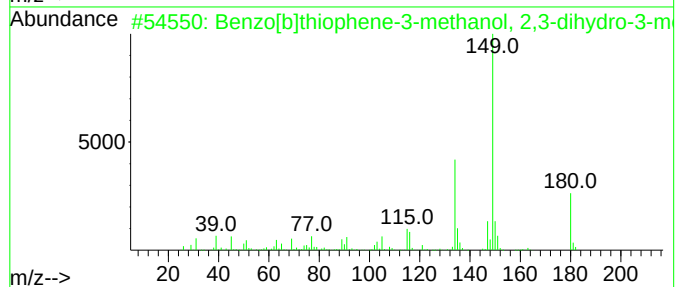
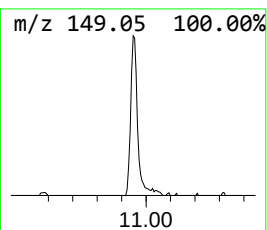
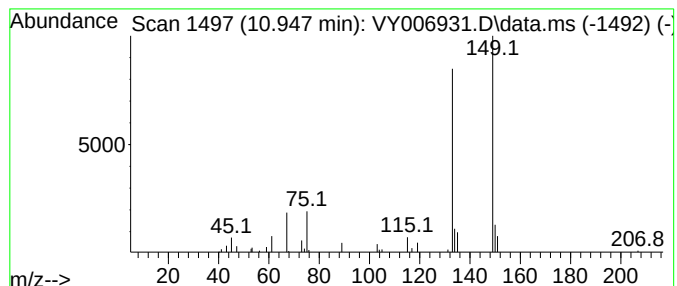
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\SFAMYL120321SMA.M
Quant Title : VOC Analysis

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

Peak Number 4 unknown-01 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.947	1.97 ug/L	30882	Chlorobenzene-d5	11.496

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[b]thiophene-3-methanol, 2,...	180	C10H12OS	039891-65-1	32
2			4-Ethylbenzoic acid, allyl ester	190	C12H14O2	1000293-31-7	32
3			2-Methoxy-3-methylbenzamide, N,N...	193	C11H15NO2	1369798-01-5	32
4			4-Ethylbenzoic acid, cyclohexyl ...	232	C15H20O2	1000293-32-1	25
5			Silane, diethoxydimethyl-	148	C6H16O2Si	000078-62-6	25



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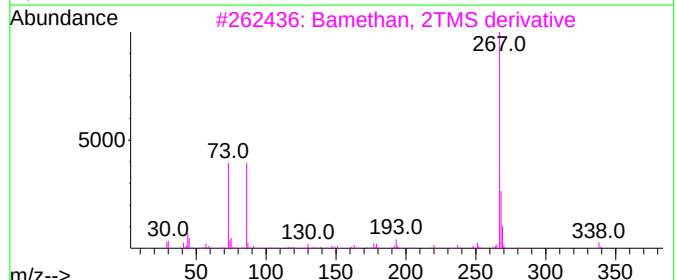
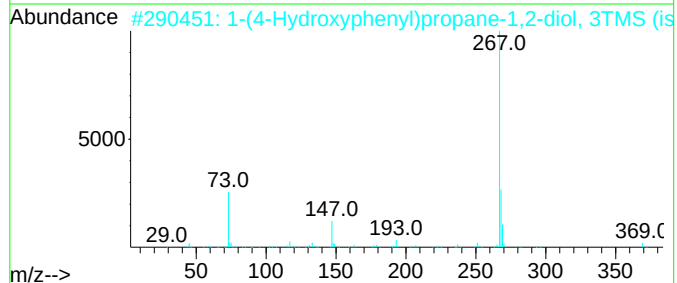
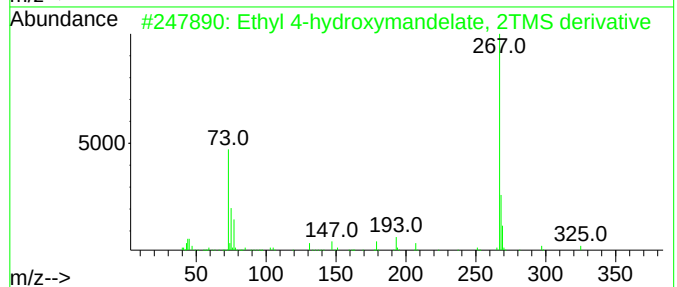
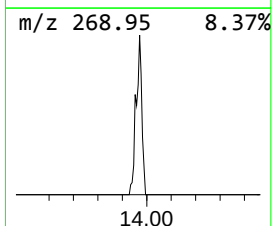
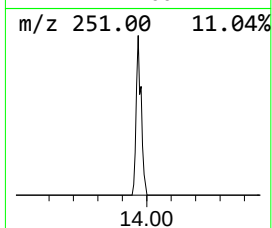
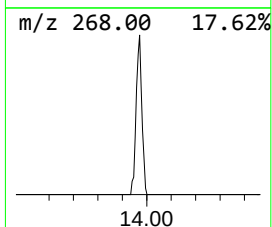
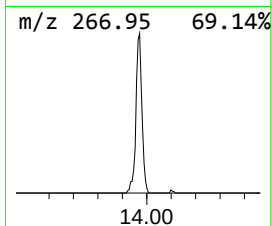
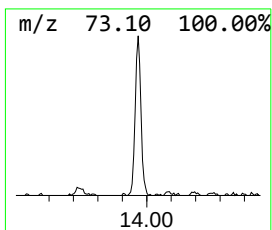
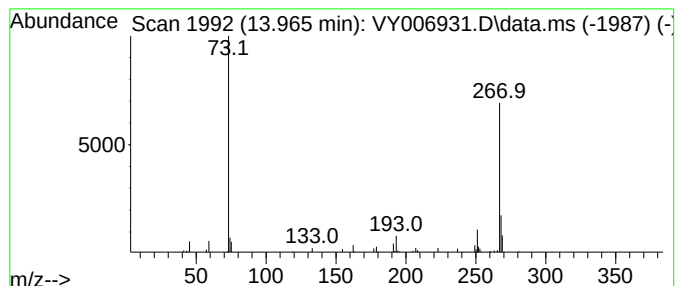
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 1-(4-Hydroxyphenyl)propane-... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.965	5.07 ug/L	38498	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethyl 4-hydroxymandelate, 2TMS d...	340	C16H28O4Si2	1010071-53-3	64
2			1-(4-Hydroxyphenyl)propane-1,2-d...	384	C18H36O3Si3	1000495-85-6	64
3			Bamethan, 2TMS derivative	353	C18H35NO2Si2	040629-66-1	64
4			4-(2-amino-1-hydroxypropyl)pheno...	311	C15H29NO2Si2	1000478-98-6	64
5			9-Acridinol, trimethylsilyl ether	267	C16H17NOSi	1000463-65-5	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	10.947	2.0	ug/L	30882	2	11.496	391129	25.0
1-(4-Hydroxyphe...	13.965	5.1	ug/L	38498	3	13.428	189839	25.0