

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY111821\
 Data File : VY006810.D
 Acq On : 18 Nov 2021 16:33
 Operator : SY/MD
 Sample : M4766-01
 Misc : 5.00G/5ML/MSVOA_Y/SOIL
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 CHRT-20058

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % 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\82Y111521S.M
 Title : SW846 8260

Signal : TIC: VY006810.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.223	61	66	73	rBV5	1240	2917	1.30%	0.206%
2	3.259	230	236	241	rVB5	1005	2424	1.08%	0.171%
3	3.954	342	350	356	rBV	1828	4505	2.01%	0.318%
4	4.210	379	392	401	rBV3	1924	5914	2.65%	0.417%
5	4.722	467	476	487	rBV3	6551	20421	9.13%	1.441%
6	5.753	636	645	655	rBV5	1570	4896	2.19%	0.345%
7	6.990	838	848	849	rBV	3614	5921	2.65%	0.418%
8	7.722	959	968	974	rBV2	29403	70647	31.60%	4.984%
9	7.795	974	980	993	rVB	55068	120208	53.76%	8.480%
10	8.142	1023	1037	1047	rVB2	39563	111869	50.03%	7.892%
11	8.691	1118	1127	1136	rBV	80316	164293	73.48%	11.590%
12	9.746	1295	1300	1310	rBV5	1530	3072	1.37%	0.217%
13	10.185	1364	1372	1380	rBV	128400	223590	100.00%	15.774%
14	10.581	1430	1437	1444	rBV	12472	21855	9.77%	1.542%
15	10.953	1492	1498	1505	rBV4	2982	5513	2.47%	0.389%
16	11.319	1552	1558	1566	rVB	11734	19570	8.75%	1.381%
17	11.489	1580	1586	1594	rBV	108187	178912	80.02%	12.622%
18	12.337	1720	1725	1729	rBV2	2055	2924	1.31%	0.206%
19	12.489	1741	1750	1758	rVB2	116729	209684	93.78%	14.793%
20	12.587	1761	1766	1770	rVB4	1762	2799	1.25%	0.197%
21	12.892	1811	1816	1822	rBV3	1680	2698	1.21%	0.190%
22	13.184	1859	1864	1870	rVB	7674	11400	5.10%	0.804%
23	13.282	1872	1880	1885	rVV6	1777	3453	1.54%	0.244%
24	13.428	1896	1904	1910	rBV	76303	117443	52.53%	8.285%
25	13.489	1910	1914	1919	rVB5	1883	3839	1.72%	0.271%
26	13.757	1952	1958	1961	rBV6	2277	4021	1.80%	0.284%
27	13.965	1986	1992	2000	rVB	12458	20743	9.28%	1.463%
28	14.257	2035	2040	2046	rBV7	2628	4767	2.13%	0.336%
29	14.422	2063	2067	2071	rVB6	1902	2688	1.20%	0.190%
30	14.471	2073	2075	2081	rVB6	2114	3664	1.64%	0.258%
31	14.617	2095	2099	2104	rBV6	2369	3701	1.66%	0.261%
32	14.678	2107	2109	2114	rVV7	1563	2551	1.14%	0.180%
33	14.733	2114	2118	2126	rVB8	2985	5365	2.40%	0.378%
34	14.849	2132	2137	2140	rBV5	2932	5342	2.39%	0.377%
35	14.940	2146	2152	2156	rVB9	3353	6134	2.74%	0.433%
36	15.038	2156	2168	2171	rBV9	3339	12056	5.39%	0.851%

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Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

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Peak separation: 5

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37	15.318	2209	2214	2222	rBV3	7726	15180	6.79%	1.071%
38	15.446	2233	2235	2239	rVB5	2891	3163	1.41%	0.223%
39	15.489	2239	2242	2245	rBV5	2305	3792	1.70%	0.268%
40	15.550	2248	2252	2253	rBV4	2572	3551	1.59%	0.251%

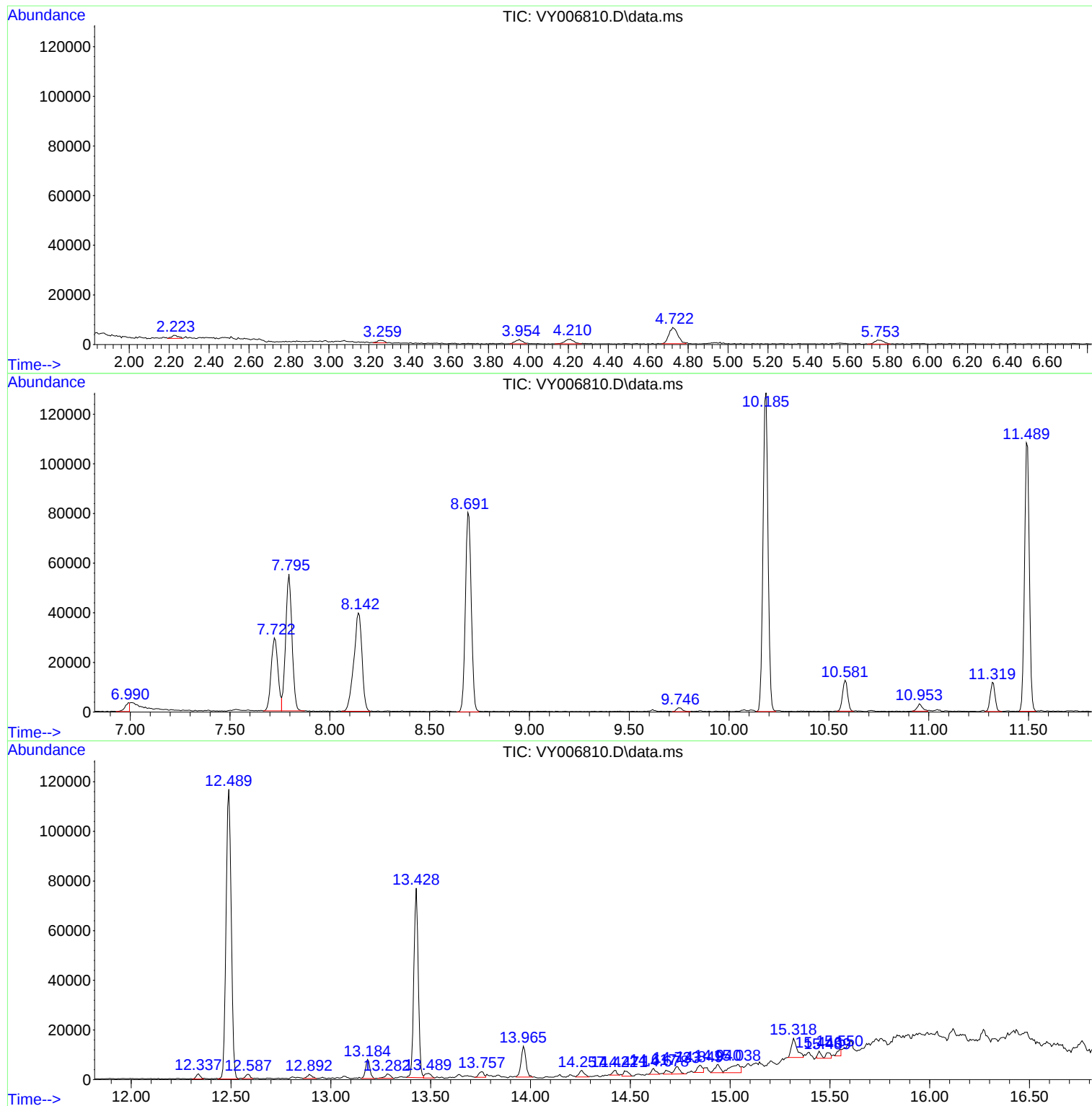
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y111521S.M
Quant Title : SW846 8260

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



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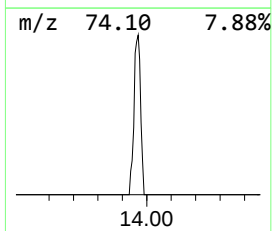
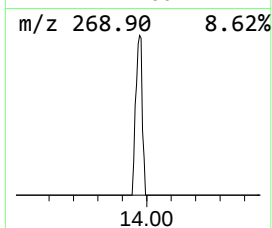
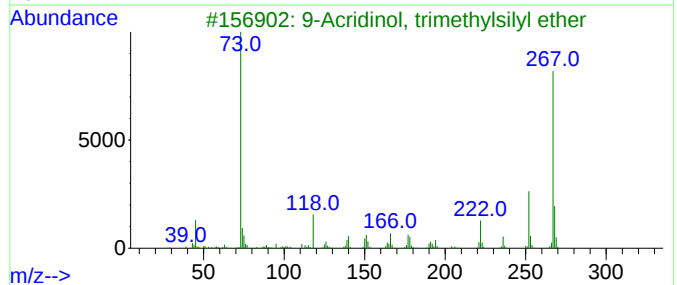
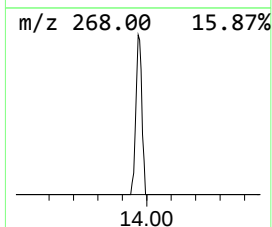
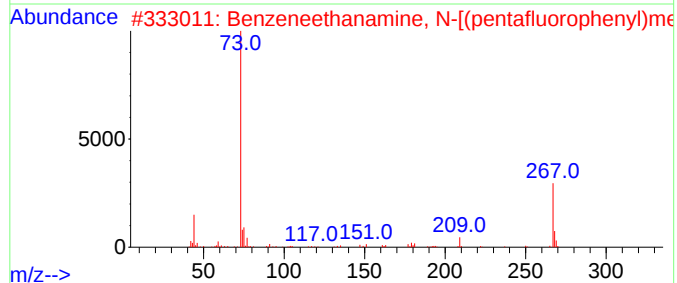
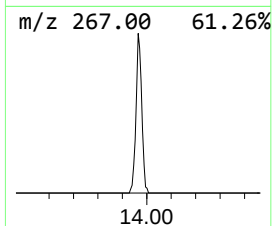
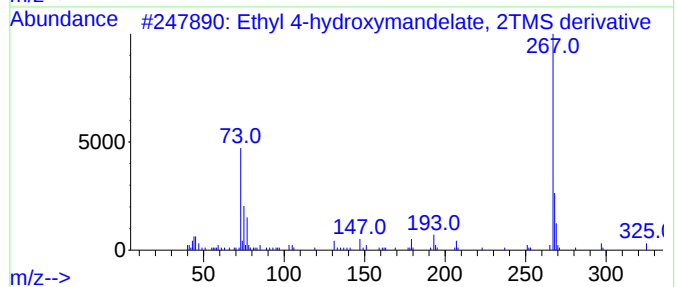
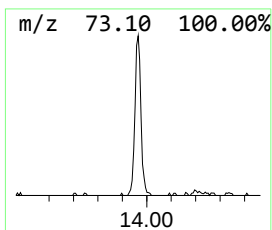
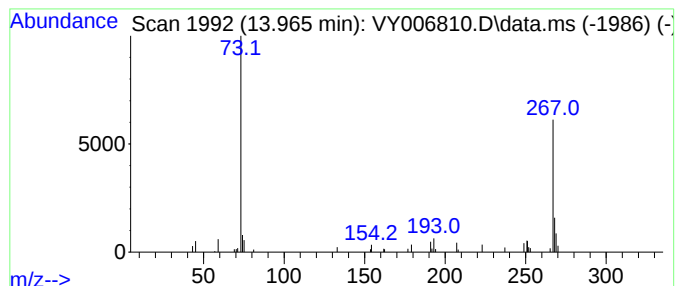
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y111521S.M
Quant Title : SW846 8260

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

Peak Number 3 Ethyl 4-hydroxymandelate, 2... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.964	8.83 ug/l	20743	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	59
2			Benzeneethanamine, N-[(pentaflu...	475	C21H26F5NO2Si2	055429-85-1	59
3			9-Acridinol, trimethylsilyl ether	267	C16H17NOSi	1000463-65-5	53
4			3-Hydroxymandelic acid, ethyl es...	340	C16H28O4Si2	1000071-88-9	50
5			2-Amino-4-methylphenol, 2TMS der...	267	C13H25NOSi2	1000373-28-1	47



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ALS Vial : 14 Sample Multiplier: 1

Instrument :
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ClientSampleId :
CHRT-20058

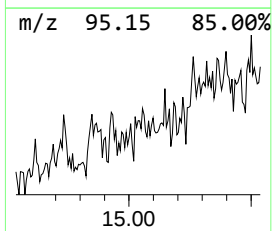
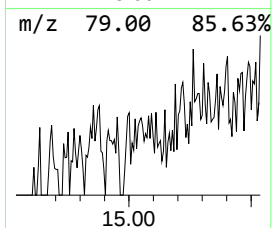
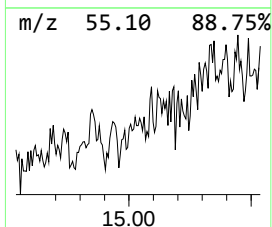
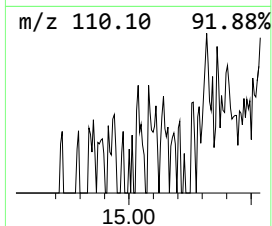
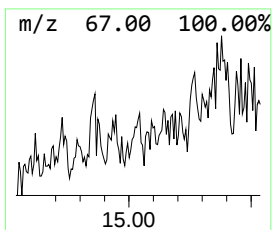
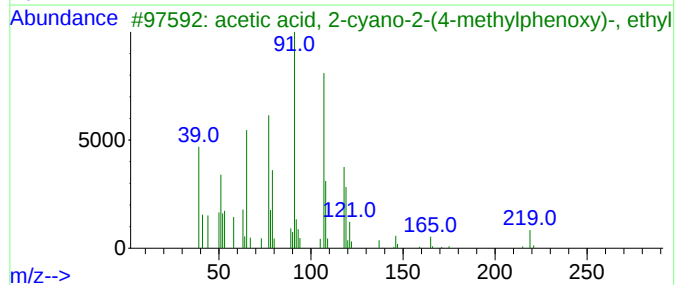
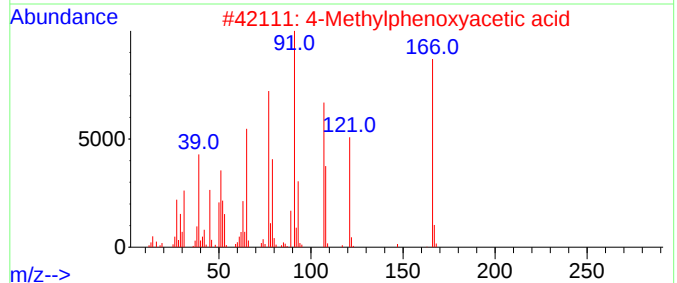
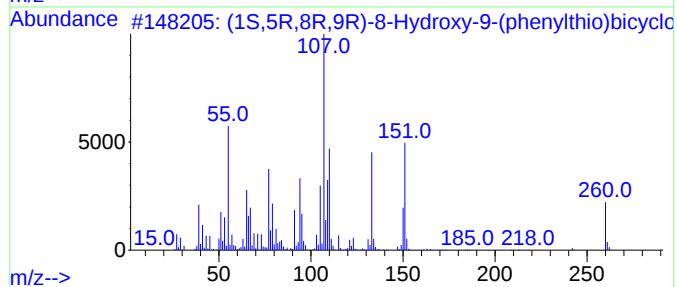
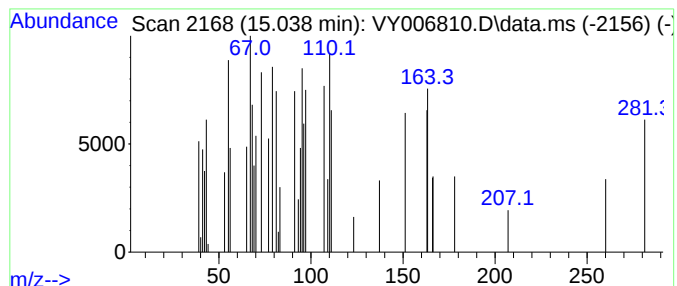
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Peak Number 4 unknown15.038 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.038	5.13 ug/l	12056	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(1S,5R,8R,9R)-8-Hydroxy-9-(pheny...	260	C15H16O2S	1000481-62-5	27		
2	4-Methylphenoxyacetic acid	166	C9H10O3	1000342-51-6	25		
3	acetic acid, 2-cyano-2-(4-methyl...	219	C12H13NO3	1000396-23-6	22		
4	3-Methylphenoxyacetic acid	166	C9H10O3	1000342-53-0	14		
5	2-Cyclohexen-1-one, 3-acetyl-5,5...	166	C10H14O2	077822-65-2	11		



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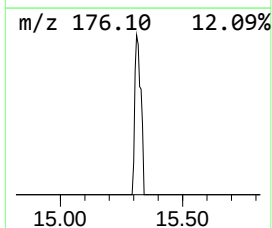
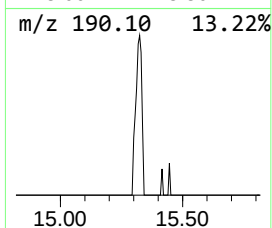
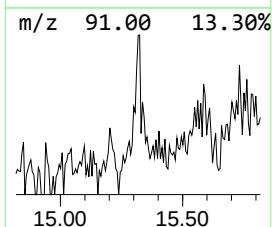
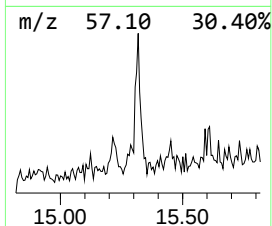
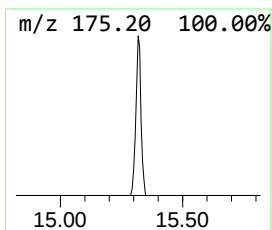
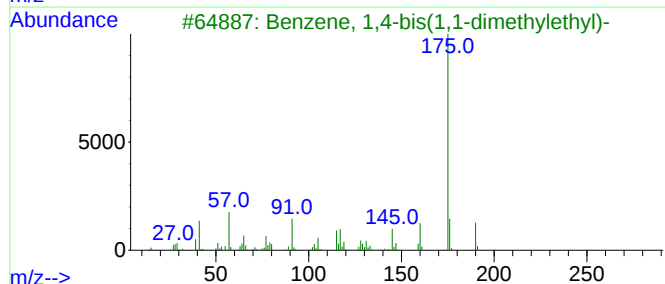
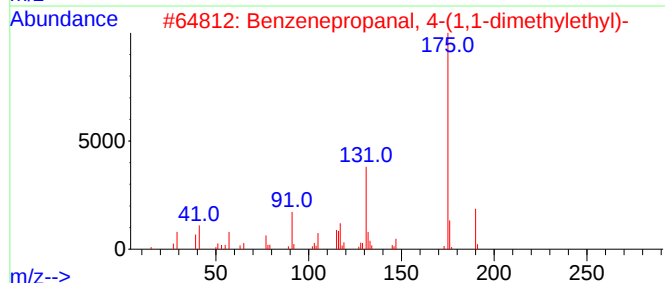
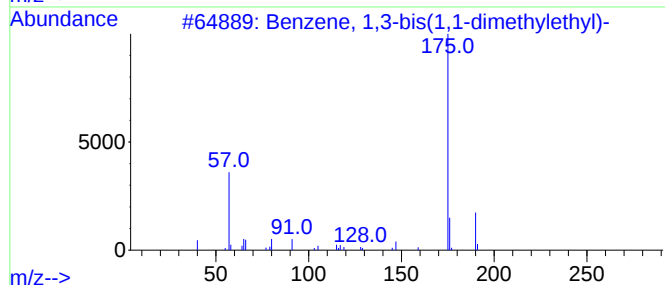
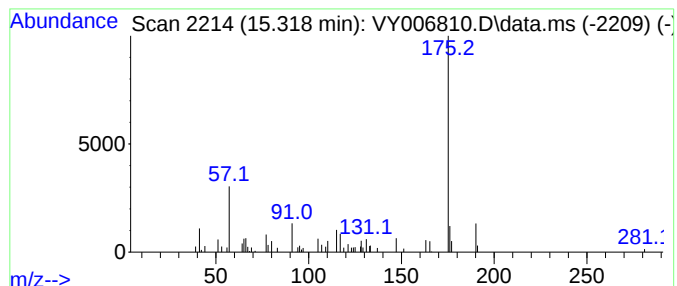
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y111521S.M
Quant Title : SW846 8260

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

Peak Number 5 Benzene, 1,3-bis(1,1-dimeth... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.318	6.46 ug/l	15180	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,3-bis(1,1-dimethyleth...	190	C14H22	001014-60-4	81
2			Benzenepropanal, 4-(1,1-dimethyl...	190	C13H18O	018127-01-0	74
3			Benzene, 1,4-bis(1,1-dimethyleth...	190	C14H22	001012-72-2	74
4			Isothiazole, 3-methyl-5-phenyl-	175	C10H9NS	001732-45-2	64
5			p-Pentylacetophenone	190	C13H18O	037593-02-5	64



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TIC Library : C:\Database\NIST20.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethyl 4-hydroxy...	13.964	8.8	ug/l	20743	4	13.428	117443	50.0
unknown15.038	15.038	5.1	ug/l	12056	4	13.428	117443	50.0
Benzene, 1,3-bi...	15.318	6.5	ug/l	15180	4	13.428	117443	50.0