

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031622\
 Data File : VX027474.D
 Acq On : 16 Mar 2022 16:27
 Operator : JC/MD
 Sample : N1950-08
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 31424

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_X\Method\82X030822W.M
 Title : SW846 8260

Signal : TIC: VX027474.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.142	6	9	16	rVB2	38479	37144	2.06%	0.277%
2	1.313	31	37	39	rVV5	17093	37453	2.08%	0.279%
3	1.355	41	44	52	rVB2	26539	50982	2.83%	0.380%
4	1.453	57	60	64	rVB	14956	19330	1.07%	0.144%
5	1.544	70	75	77	rBV6	13492	23195	1.29%	0.173%
6	2.215	181	185	193	rVB4	16658	36016	2.00%	0.268%
7	2.380	208	212	223	rVB	31228	54048	3.00%	0.403%
8	2.538	231	238	245	rBV	14028	26382	1.47%	0.197%
9	5.391	694	706	722	rBV	223076	646047	35.88%	4.812%
10	5.556	722	733	748	rVB	374332	1064055	59.10%	7.926%
11	5.958	787	799	817	rBV	220943	591474	32.85%	4.406%
12	6.641	901	911	920	rBV2	29312	75662	4.20%	0.564%
13	6.763	922	931	947	rVB	555004	1344204	74.66%	10.012%
14	6.958	956	963	976	rBV2	20240	51871	2.88%	0.386%
15	7.903	1113	1118	1131	rVB	22988	46551	2.59%	0.347%
16	8.653	1233	1241	1249	rBV	1166786	1800426	100.00%	13.410%
17	8.805	1261	1266	1273	rBV	22095	36948	2.05%	0.275%
18	9.244	1333	1338	1347	rBV	57298	88350	4.91%	0.658%
19	9.445	1364	1371	1379	rBV	15956	28014	1.56%	0.209%
20	9.835	1431	1435	1442	rVB	19419	26524	1.47%	0.198%
21	9.945	1446	1453	1461	rBV	56573	82511	4.58%	0.615%
22	10.055	1461	1471	1484	rBV	1232718	1616185	89.77%	12.038%
23	10.213	1489	1497	1503	rBV	28025	45504	2.53%	0.339%
24	10.274	1503	1507	1511	rBV2	16773	22557	1.25%	0.168%
25	10.872	1598	1605	1615	rBV3	25852	71051	3.95%	0.529%
26	11.085	1633	1640	1650	rVV	985480	1297889	72.09%	9.667%
27	11.238	1660	1665	1669	rBV2	13841	22900	1.27%	0.171%
28	11.463	1698	1702	1709	rVB	26885	41737	2.32%	0.311%
29	11.750	1744	1749	1754	rBV2	45904	60100	3.34%	0.448%
30	11.908	1767	1775	1780	rBV4	13003	23670	1.31%	0.176%
31	11.975	1780	1786	1789	rBV	203937	268384	14.91%	1.999%
32	12.024	1789	1794	1801	rVB	1262303	1512537	84.01%	11.266%
33	12.122	1806	1810	1820	rVB2	20905	37100	2.06%	0.276%
34	12.359	1839	1849	1857	rVB	59478	111401	6.19%	0.830%
35	12.920	1934	1941	1944	rBV7	10643	19994	1.11%	0.149%
36	12.993	1950	1953	1954	rBV	19714	18545	1.03%	0.138%

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If leading or trailing edge < 100 prefer < Baseline drop else tangent >

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 Title : SW846 8260

37	13.061	1960	1964	1967	rBV	46025	58153	3.23%	0.433%
38	13.134	1971	1976	1980	rVB3	22358	31117	1.73%	0.232%
39	13.201	1983	1987	1991	rBV2	17907	24088	1.34%	0.179%
40	13.304	1999	2004	2009	rVB5	28630	55100	3.06%	0.410%
41	13.378	2012	2016	2020	rBV3	21725	34959	1.94%	0.260%
42	13.426	2020	2024	2030	rVB	35434	49806	2.77%	0.371%
43	13.481	2030	2033	2040	rVB3	11932	21481	1.19%	0.160%
44	13.585	2047	2050	2053	rBV3	16895	27614	1.53%	0.206%
45	13.621	2053	2056	2061	rVB	24680	36260	2.01%	0.270%
46	13.695	2066	2068	2072	rVB2	18126	20128	1.12%	0.150%
47	13.804	2079	2086	2091	rBV6	9797	25364	1.41%	0.189%
48	14.225	2150	2155	2158	rBV5	16209	29456	1.64%	0.219%
49	14.329	2168	2172	2183	rBV	58037	124027	6.89%	0.924%
50	14.530	2201	2205	2207	rBV	89250	111073	6.17%	0.827%
51	14.566	2207	2211	2221	rVB	170278	292638	16.25%	2.180%
52	14.719	2233	2236	2240	rVB3	40033	51098	2.84%	0.381%
53	14.792	2245	2248	2250	rVV	22985	30076	1.67%	0.224%
54	14.829	2250	2254	2262	rVV2	118589	199183	11.06%	1.484%
55	14.908	2263	2267	2270	rVV	61267	97383	5.41%	0.725%
56	14.957	2271	2275	2279	rVV2	150056	239494	13.30%	1.784%
57	14.993	2279	2281	2287	rVB	51113	63022	3.50%	0.469%
58	15.146	2300	2306	2317	rBV2	164657	360104	20.00%	2.682%
59	15.292	2323	2330	2334	rBV2	57461	107226	5.96%	0.799%

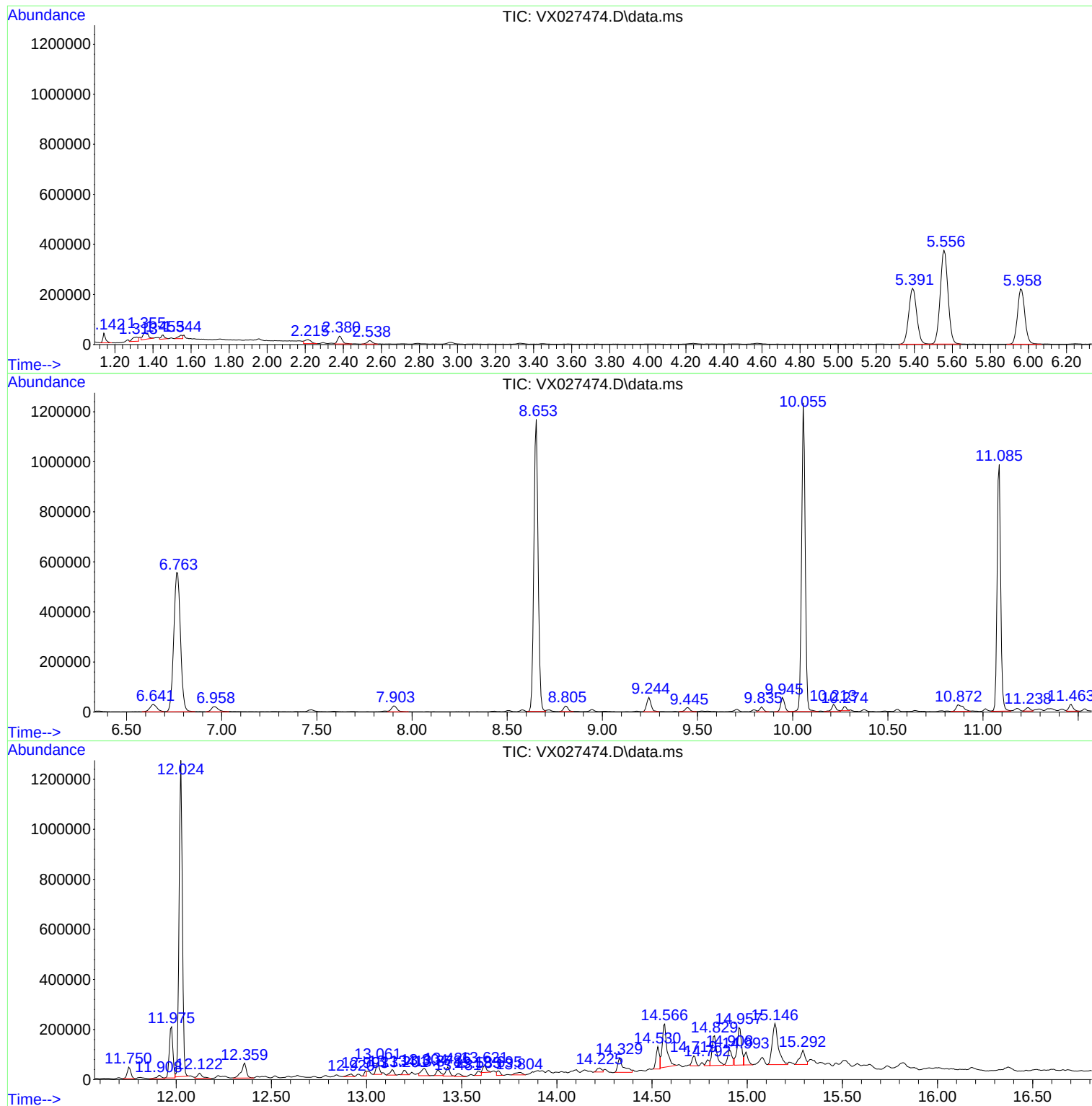
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Quant Title : SW846 8260

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



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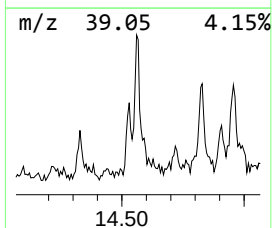
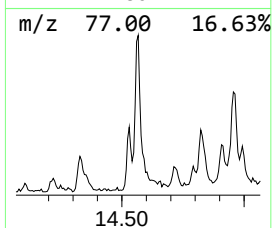
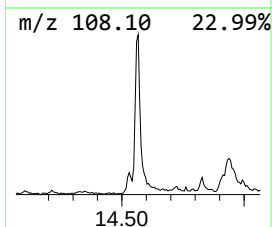
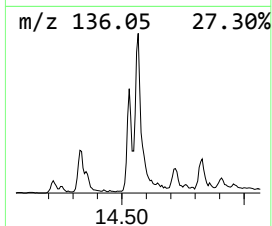
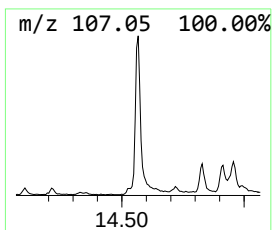
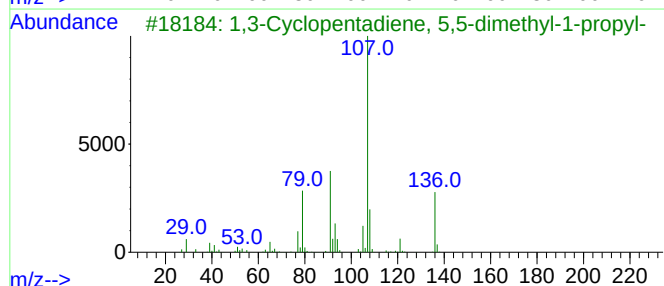
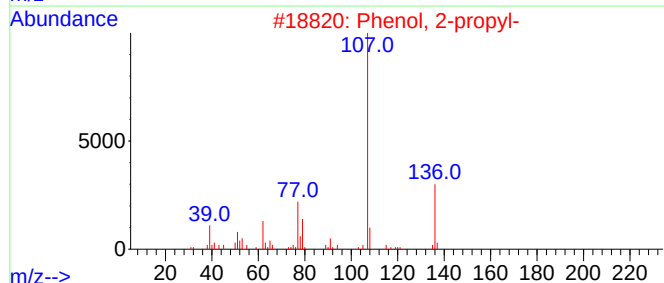
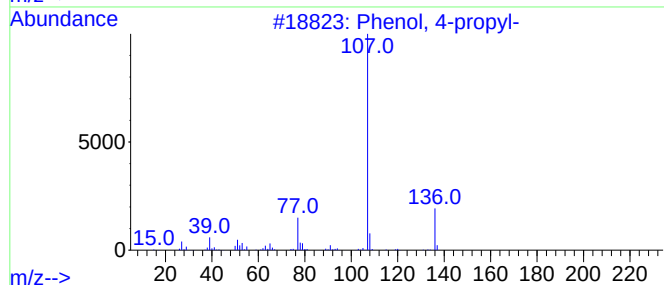
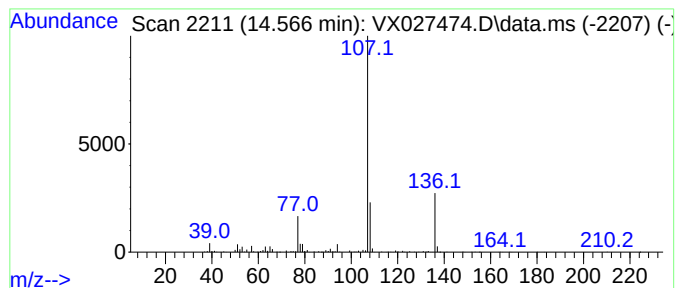
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X030822W.M
Quant Title : SW846 8260

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

Peak Number 1 Phenol, 4-propyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.566	9.67 ug/l	292638	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 4-propyl-	136	C9H12O	000645-56-7	80
2			Phenol, 2-propyl-	136	C9H12O	000644-35-9	72
3			1,3-Cyclopentadiene, 5,5-dimethy...	136	C10H16	1000163-57-1	50
4			Hydrazine, 1-ethyl-2-phenyl-	136	C8H12N2	000622-82-2	37
5			Benzenemethanol, .alpha.-2-cyclo...	188	C13H16O	005723-89-7	33



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Instrument :
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ClientSampleId :
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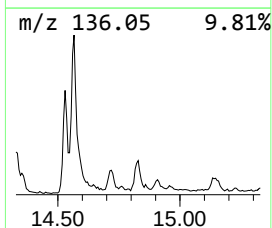
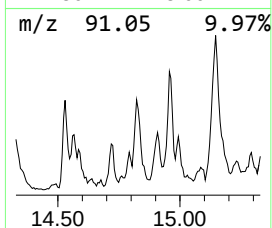
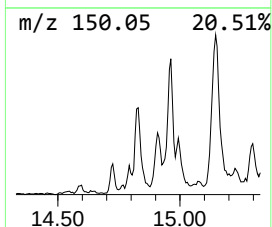
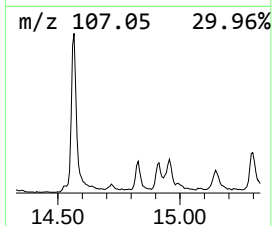
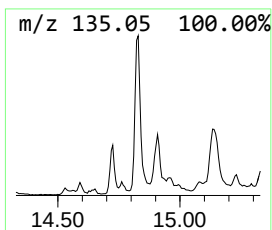
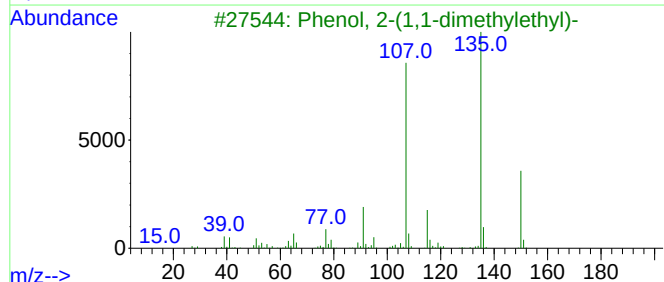
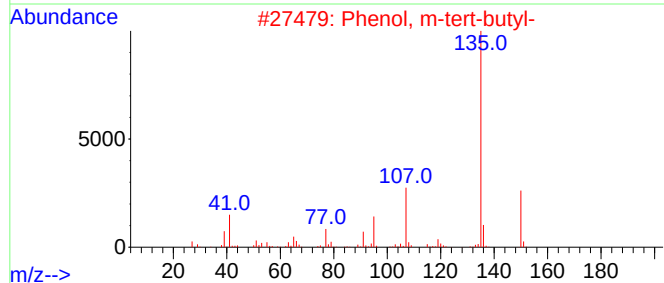
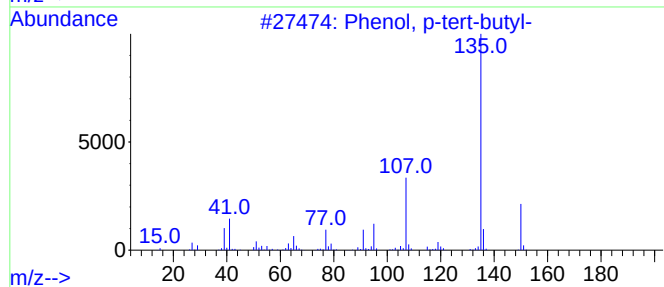
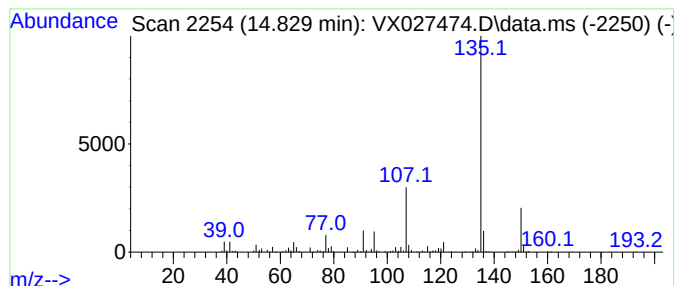
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X030822W.M
Quant Title : SW846 8260

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

Peak Number 2 Phenol, p-tert-butyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.829	6.58 ug/l	199183	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	93
2			Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	90
3			Phenol, 2-(1,1-dimethylethyl)-	150	C10H14O	000088-18-6	72
4			Phenol, 2-methyl-5-(1-methylethyl)-	150	C10H14O	000499-75-2	72
5			Hexestrol	270	C18H22O2	000084-16-2	53



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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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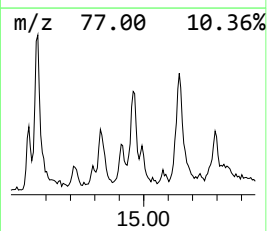
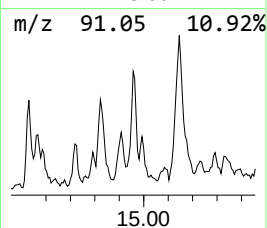
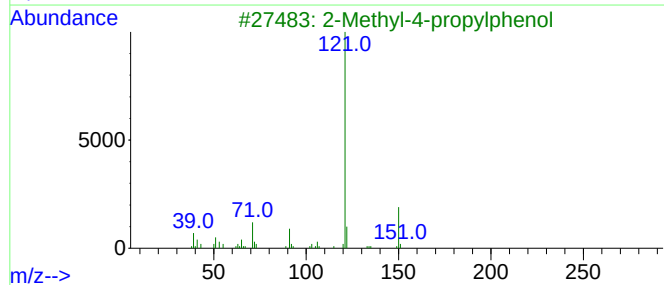
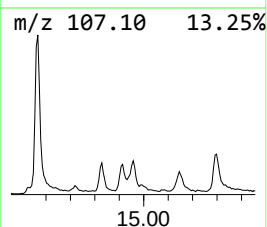
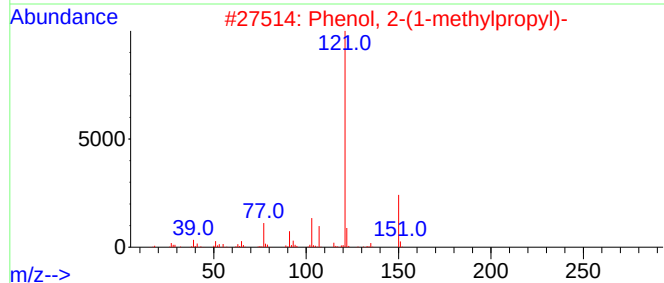
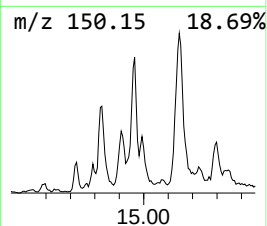
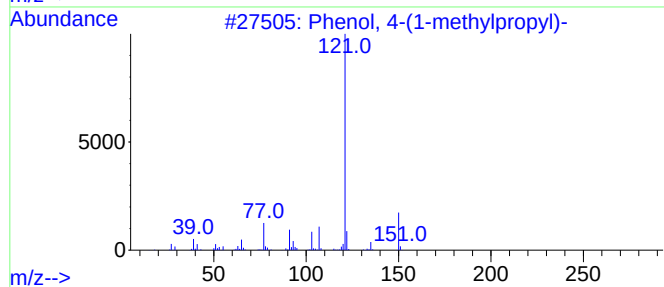
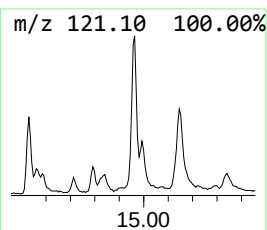
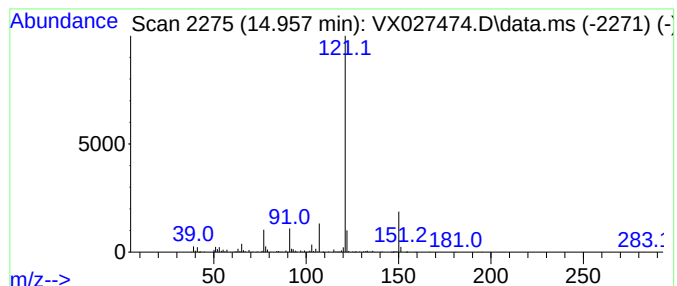
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X030822W.M
Quant Title : SW846 8260

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

Peak Number 3 Phenol, 4-(1-methylpropyl)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.957	7.92 ug/l	239494	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 4-(1-methylpropyl)-	150	C10H14O	000099-71-8	91
2			Phenol, 2-(1-methylpropyl)-	150	C10H14O	000089-72-5	86
3			2-Methyl-4-propylphenol	150	C10H14O	018441-56-0	80
4			2-Methyl-6-propylphenol	150	C10H14O	003520-52-3	78
5			Fenobucarb	207	C12H17NO2	003766-81-2	78



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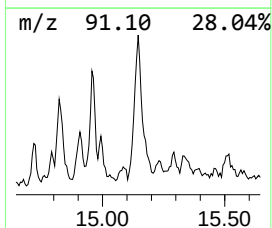
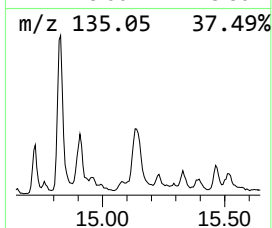
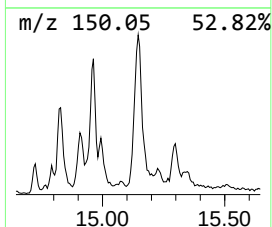
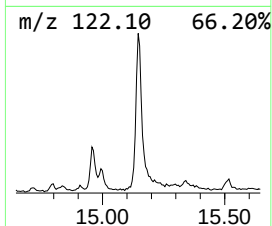
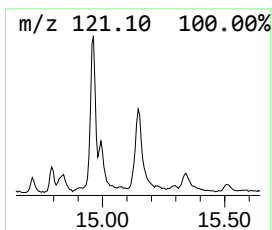
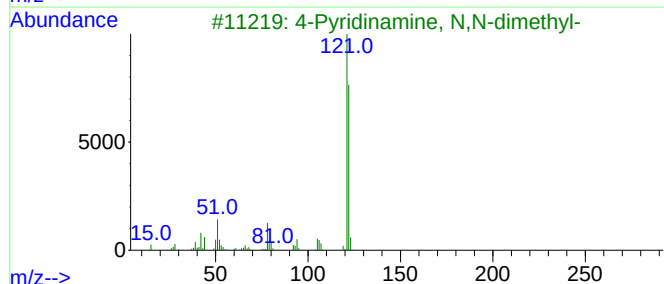
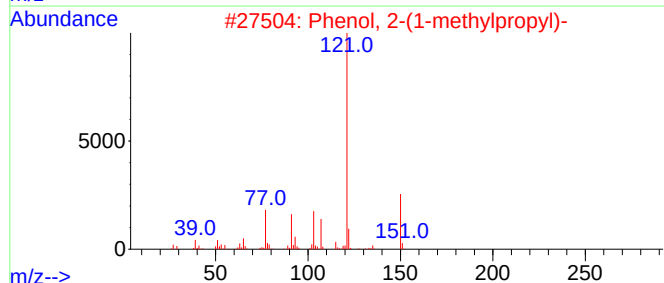
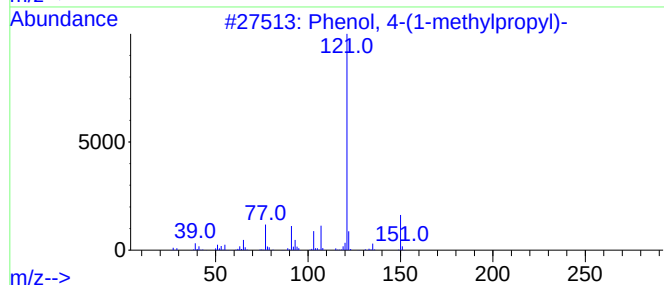
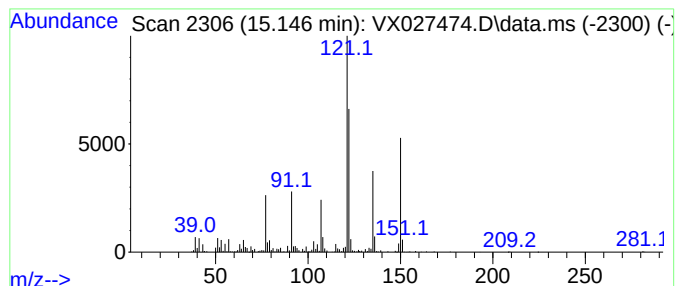
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X030822W.M
Quant Title : SW846 8260

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

Peak Number 4 Phenol, 2-(1-methylpropyl)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.146	11.90 ug/l	360104	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 4-(1-methylpropyl)-	150	C10H14O	000099-71-8	52
2			Phenol, 2-(1-methylpropyl)-	150	C10H14O	000089-72-5	52
3			4-Pyridinamine, N,N-dimethyl-	122	C7H10N2	001122-58-3	43
4			Phenol, 4-ethyl-3-methyl-	136	C9H12O	001123-94-0	41
5			Phenol, 2-ethyl-4-methyl-	136	C9H12O	003855-26-3	38



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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
Phenol, 4-propyl-	14.566	9.7	ug/l	292638	4	12.024	1512540	50.0
Phenol, p-tert-...	14.829	6.6	ug/l	199183	4	12.024	1512540	50.0
Phenol, 4-(1-me...	14.957	7.9	ug/l	239494	4	12.024	1512540	50.0
Phenol, 2-(1-me...	15.146	11.9	ug/l	360104	4	12.024	1512540	50.0