

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031522\
 Data File : VX027460.D
 Acq On : 15 Mar 2022 20:17
 Operator : JC/MD
 Sample : N1950-10
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 3222

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: VX027460.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.313	31	37	40	rBV5	24576	64450	3.67%	0.294%
2	1.453	56	60	66	rBV	58136	65044	3.71%	0.297%
3	2.057	154	159	172	rVB	146537	231236	13.18%	1.055%
4	2.380	207	212	226	rVB	18884	32725	1.87%	0.149%
5	2.538	229	238	246	rBV2	22488	50284	2.87%	0.230%
6	5.391	694	706	722	rBV2	218664	633178	36.10%	2.890%
7	5.556	722	733	752	rVB	372506	1042993	59.46%	4.761%
8	5.958	784	799	811	rBV	216667	584349	33.31%	2.667%
9	6.763	922	931	945	rBV	568211	1358263	77.43%	6.200%
10	8.653	1234	1241	1248	rBV	1131406	1754173	100.00%	8.007%
11	8.720	1248	1252	1258	rVB	14653	24878	1.42%	0.114%
12	10.055	1465	1471	1484	rBV	1173031	1548457	88.27%	7.068%
13	10.305	1507	1512	1520	rVB	13710	20999	1.20%	0.096%
14	10.403	1523	1528	1540	rVB	26137	39422	2.25%	0.180%
15	10.646	1562	1568	1574	rBV	34598	48014	2.74%	0.219%
16	11.085	1634	1640	1646	rBV	928029	1202762	68.57%	5.490%
17	11.573	1716	1720	1724	rBV	29576	36991	2.11%	0.169%
18	12.024	1789	1794	1801	rBV	1177024	1434170	81.76%	6.546%
19	12.091	1801	1805	1810	rVB	15625	23670	1.35%	0.108%
20	12.219	1822	1826	1828	rBV	36184	46039	2.62%	0.210%
21	12.250	1828	1831	1838	rVV2	26042	42586	2.43%	0.194%
22	12.616	1887	1891	1894	rBV	16595	18956	1.08%	0.087%
23	12.701	1901	1905	1913	rVB2	18804	31323	1.79%	0.143%
24	12.927	1936	1942	1946	rVV2	25580	52670	3.00%	0.240%
25	13.170	1978	1982	1992	rVB2	30425	53683	3.06%	0.245%
26	13.292	1997	2002	2008	rVV2	74221	102964	5.87%	0.470%
27	13.426	2019	2024	2029	rVB	24696	33871	1.93%	0.155%
28	13.548	2040	2044	2046	rVV	22105	28459	1.62%	0.130%
29	13.585	2046	2050	2055	rVV3	35244	54050	3.08%	0.247%
30	13.658	2056	2062	2071	rVB3	73551	138139	7.87%	0.631%
31	13.896	2089	2101	2104	rBV2	134378	357485	20.38%	1.632%
32	13.926	2104	2106	2111	rVV3	52825	80213	4.57%	0.366%
33	13.975	2111	2114	2117	rVV	22262	30356	1.73%	0.139%
34	14.079	2126	2131	2133	rBV	51263	68424	3.90%	0.312%
35	14.103	2133	2135	2141	rVB	38033	42355	2.41%	0.193%
36	14.219	2147	2154	2158	rBV3	176111	309803	17.66%	1.414%

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37	14.329	2167	2172	2184	rBV	459149	915945	52.22%	4.181%
38	14.481	2192	2197	2201	rBV2	50331	71800	4.09%	0.328%
39	14.530	2201	2205	2207	rBV	433362	542002	30.90%	2.474%
40	14.567	2207	2211	2221	rVB	783482	1382702	78.82%	6.311%
41	14.725	2232	2237	2241	rBV2	271625	388803	22.16%	1.775%
42	14.786	2241	2247	2250	rVV2	444158	738460	42.10%	3.371%
43	14.823	2250	2253	2262	rVV3	633790	1045800	59.62%	4.773%
44	14.908	2262	2267	2271	rVV	326727	561662	32.02%	2.564%
45	14.963	2271	2276	2279	rVV	789408	1215903	69.31%	5.550%
46	14.993	2279	2281	2292	rVB	316390	415560	23.69%	1.897%
47	15.079	2292	2295	2300	rBV5	40202	78181	4.46%	0.357%
48	15.146	2300	2306	2317	rBV3	336573	850553	48.49%	3.882%
49	15.225	2317	2319	2323	rVB	23431	24366	1.39%	0.111%
50	15.268	2323	2326	2328	rBV3	38268	56173	3.20%	0.256%
51	15.292	2328	2330	2333	rVB2	47211	50872	2.90%	0.232%
52	15.335	2333	2337	2341	rVB2	84275	113251	6.46%	0.517%
53	15.396	2342	2347	2355	rVB6	89142	210904	12.02%	0.963%
54	15.475	2355	2360	2364	rBV2	248306	444132	25.32%	2.027%
55	15.572	2373	2376	2379	rBV4	20351	27534	1.57%	0.126%
56	15.615	2379	2383	2386	rBV	273237	372495	21.23%	1.700%
57	15.652	2386	2389	2397	rVB2	154139	241523	13.77%	1.102%
58	15.737	2399	2403	2408	rVB4	26981	44386	2.53%	0.203%
59	15.816	2409	2416	2417	rBV7	64780	117877	6.72%	0.538%
60	15.993	2440	2445	2452	rVB	43565	78138	4.45%	0.357%
61	16.328	2495	2500	2504	rBV	68700	134490	7.67%	0.614%
62	16.481	2521	2525	2530	rVB6	11430	19276	1.10%	0.088%
63	16.603	2541	2545	2550	rVB2	24493	40700	2.32%	0.186%
64	16.658	2550	2554	2557	rBV3	20853	38098	2.17%	0.174%

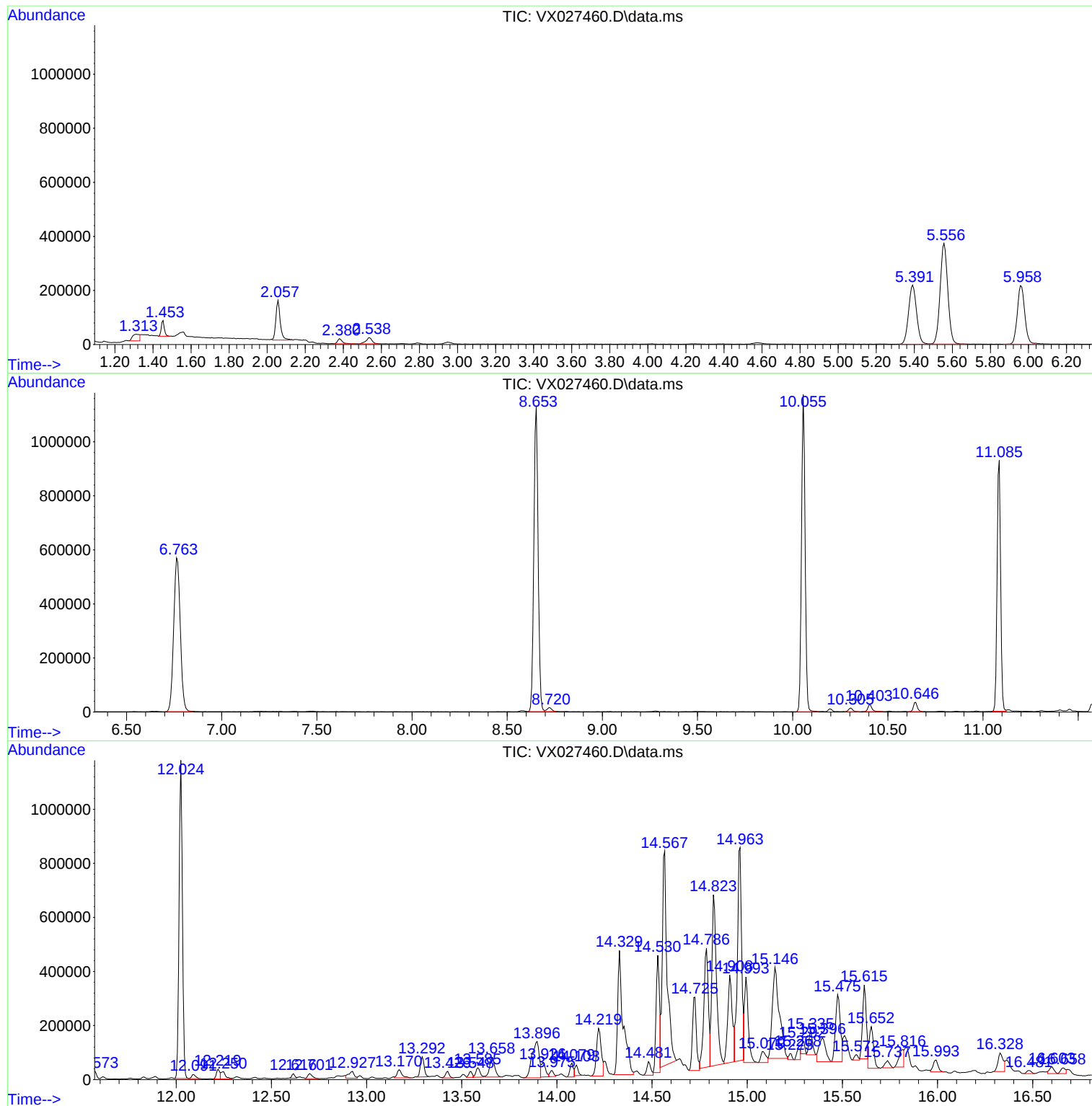
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X030822W.M
Quant Title : SW846 8260

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



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ClientSampleId :
3222

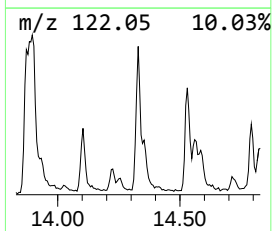
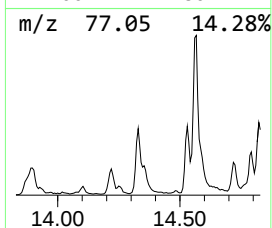
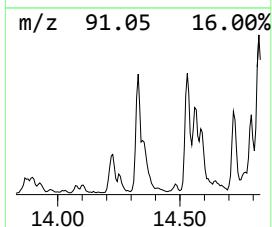
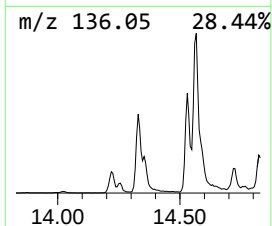
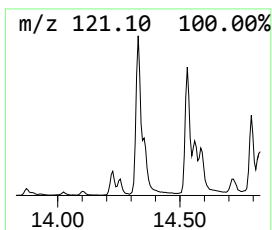
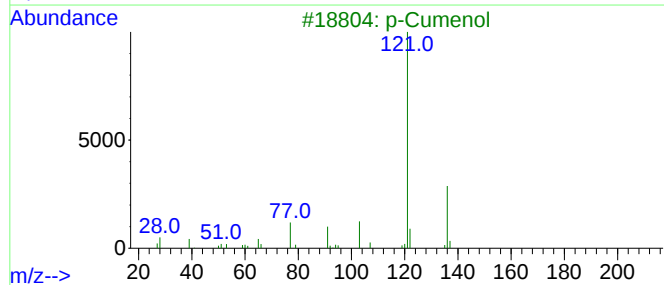
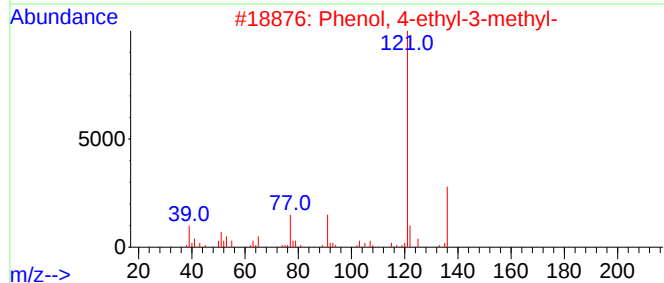
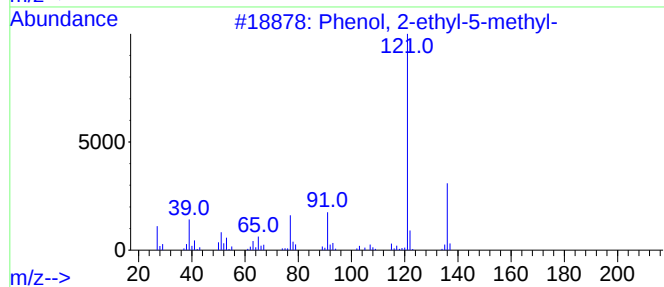
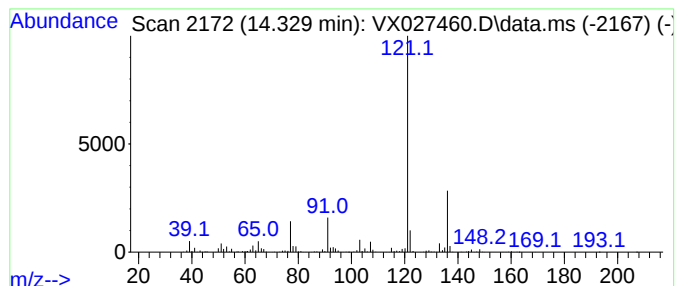
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X030822W.M
Quant Title : SW846 8260

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

Peak Number 1 Phenol, 2-ethyl-5-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.329	31.93 ug/l	915945	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 2-ethyl-5-methyl-	136	C9H12O	001687-61-2	90
2			Phenol, 4-ethyl-3-methyl-	136	C9H12O	001123-94-0	90
3			p-Cumenol	136	C9H12O	000099-89-8	90
4			Phenol, 3-ethyl-5-methyl-	136	C9H12O	000698-71-5	87
5			Phenol, 3-(1-methylethyl)-	136	C9H12O	000618-45-1	87



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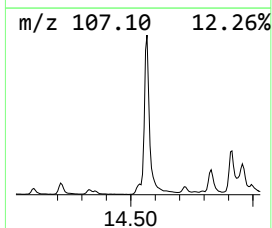
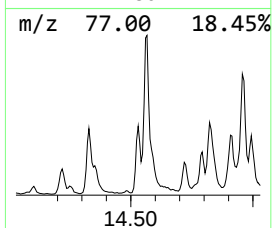
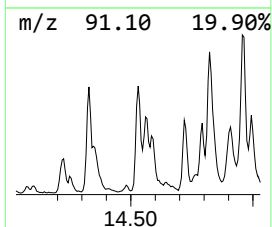
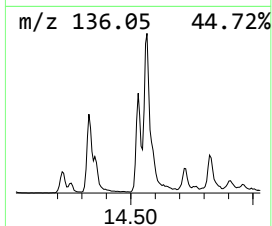
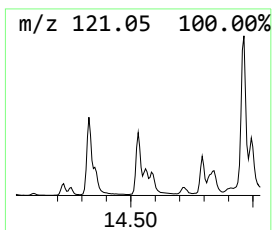
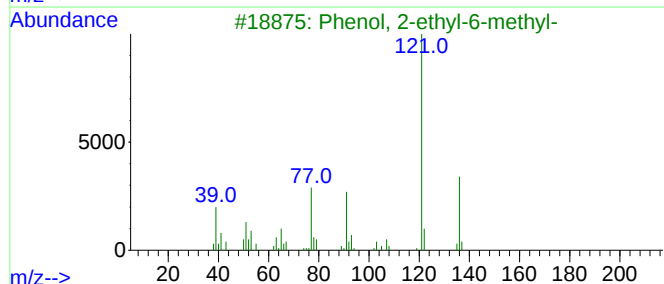
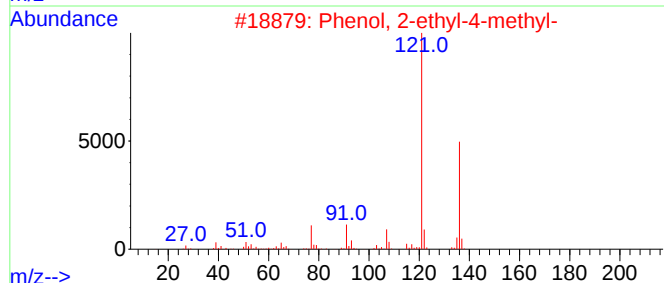
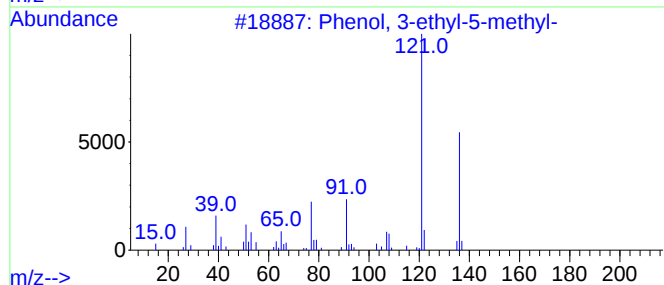
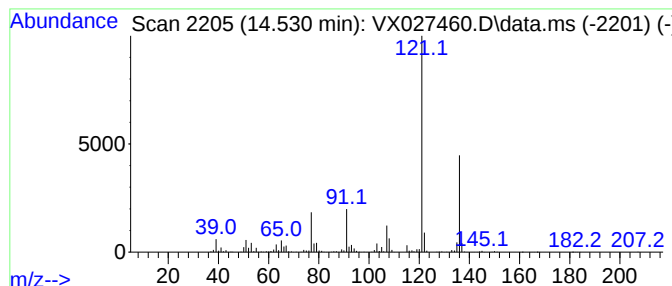
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X030822W.M
Quant Title : SW846 8260

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

Peak Number 2 Phenol, 3-ethyl-5-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.530	18.90 ug/l	542002	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 3-ethyl-5-methyl-	136	C9H12O	000698-71-5	94
2			Phenol, 2-ethyl-4-methyl-	136	C9H12O	003855-26-3	91
3			Phenol, 2-ethyl-6-methyl-	136	C9H12O	001687-64-5	91
4			Phenol, 2-ethyl-5-methyl-	136	C9H12O	001687-61-2	90
5			Phenol, 3-(1-methylethyl)-	136	C9H12O	000618-45-1	86



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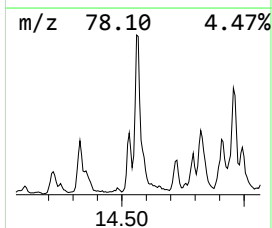
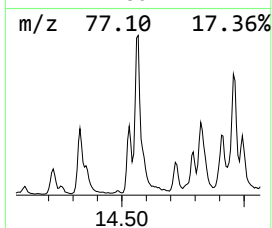
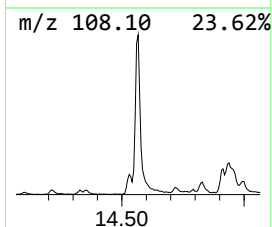
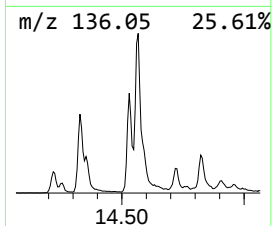
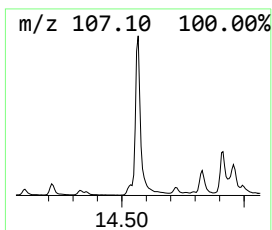
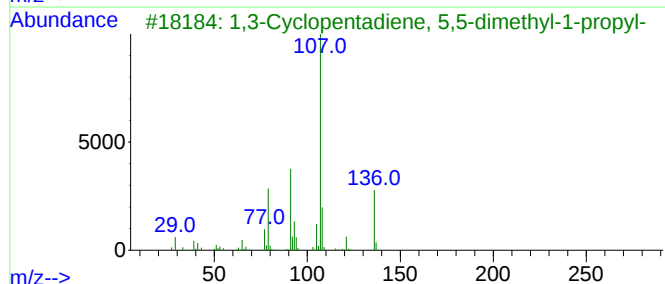
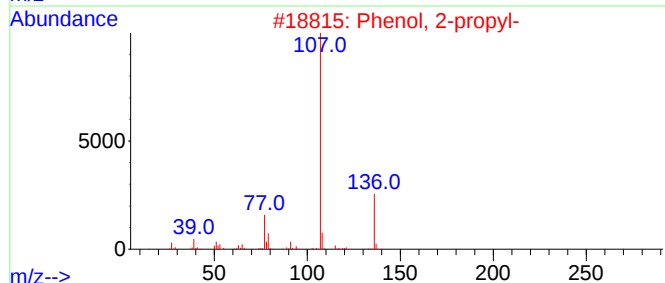
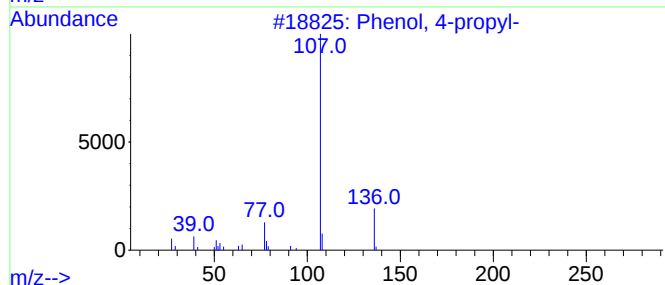
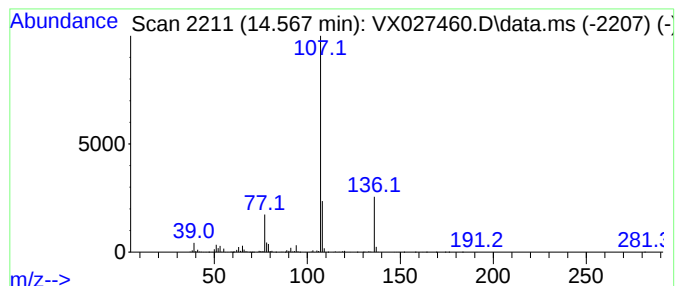
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Quant Title : SW846 8260

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

Peak Number 3 Phenol, 4-propyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.567	48.21 ug/l	1382700	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 4-propyl-	136	C9H12O	000645-56-7	83
2			Phenol, 2-propyl-	136	C9H12O	000644-35-9	74
3			1,3-Cyclopentadiene, 5,5-dimethy...	136	C10H16	1000163-57-1	64
4			Phenol, 4-ethyl-	122	C8H10O	000123-07-9	42
5			Benzenemethanol, .alpha.-2-cyclo...	188	C13H16O	005723-89-7	33



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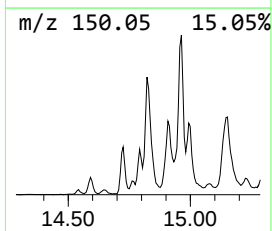
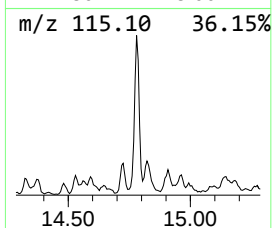
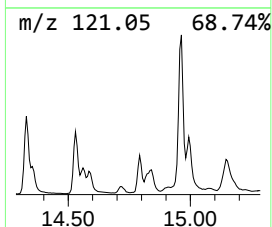
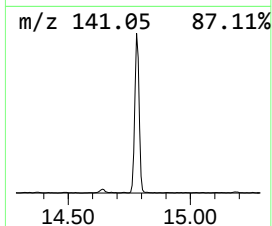
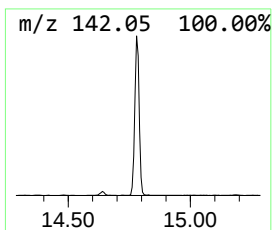
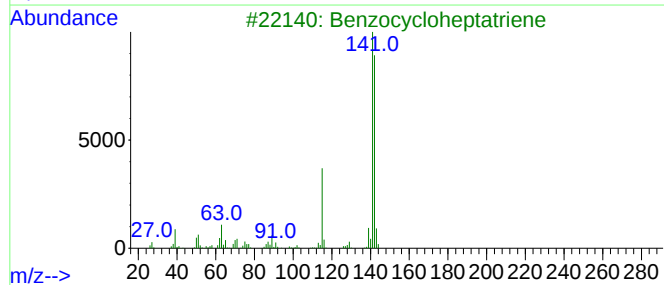
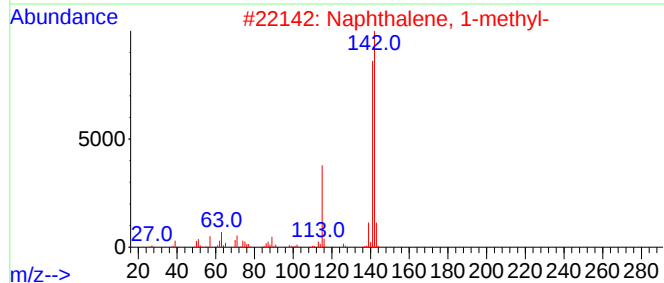
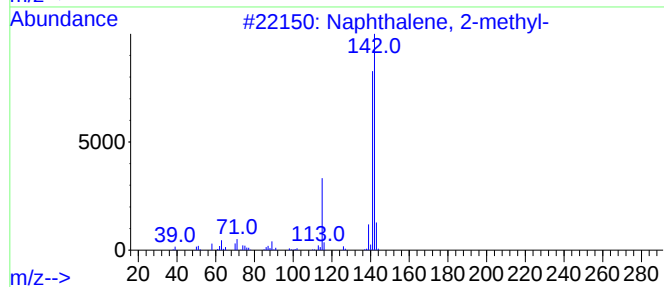
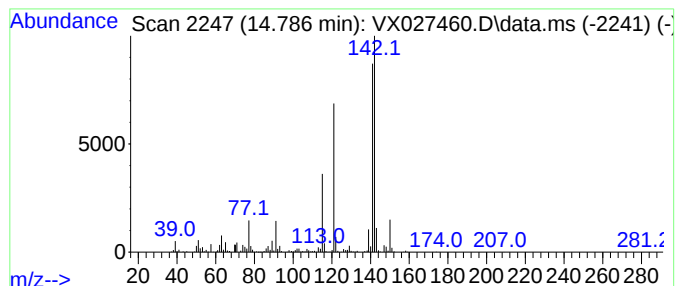
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X030822W.M
Quant Title : SW846 8260

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

Peak Number 4 Benzocycloheptatriene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.786	25.75 ug/l	738460	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3			Benzocycloheptatriene	142	C11H10	000264-09-5	90
4			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	87
5			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	74



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ClientSampleId :
3222

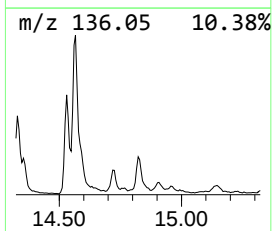
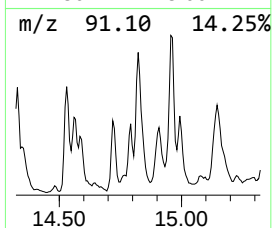
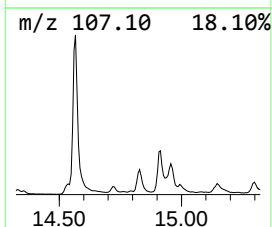
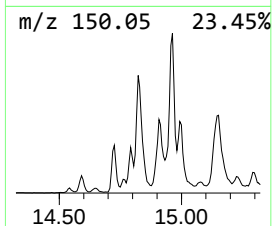
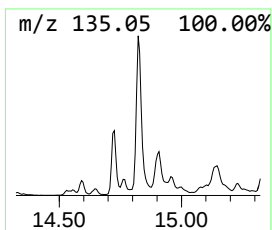
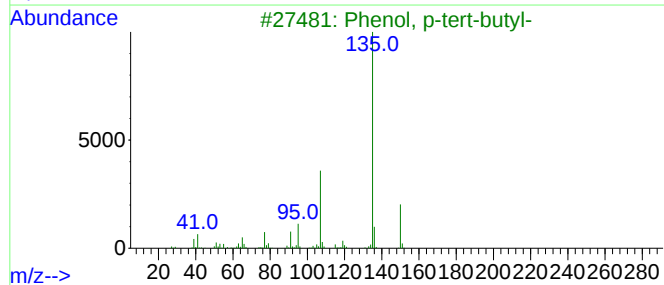
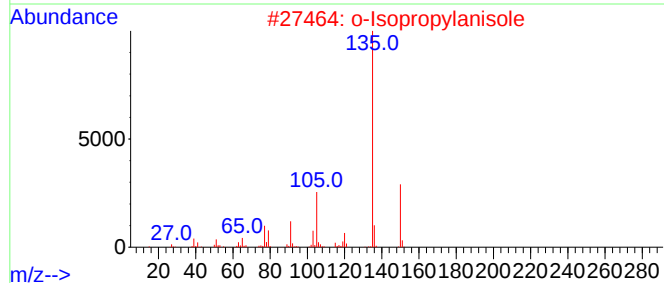
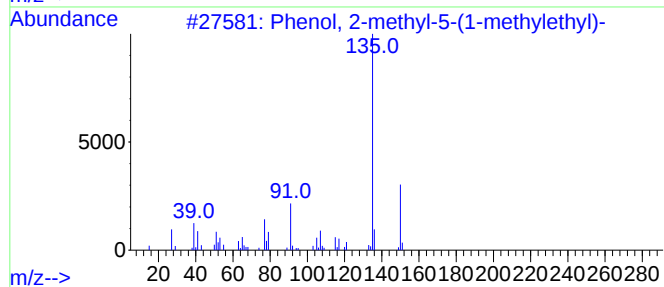
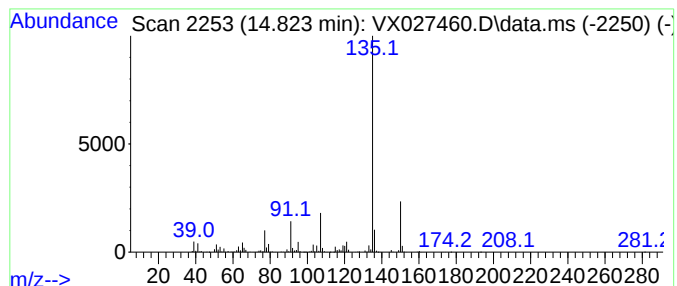
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Quant Title : SW846 8260

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

Peak Number 5 Phenol, 2-methyl-5-(1-methy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.823	36.46 ug/l	1045800	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 2-methyl-5-(1-methylethyl)-	150	C10H14O	000499-75-2	87
2			o-Isopropylanisole	150	C10H14O	002944-47-0	80
3			Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	80
4			Thymol	150	C10H14O	000089-83-8	80
5			3-Methyl-4-isopropylphenol	150	C10H14O	003228-02-2	80



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031522\
Data File : VX027460.D
Acq On : 15 Mar 2022 20:17
Operator : JC/MD
Sample : N1950-10
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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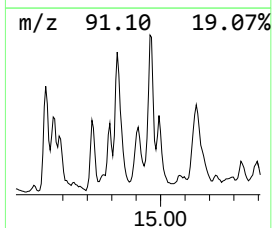
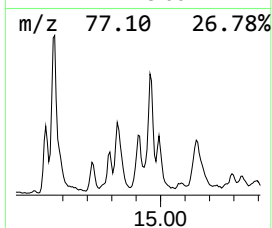
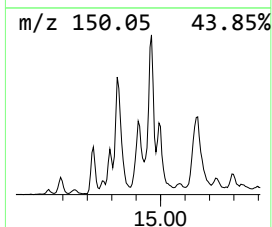
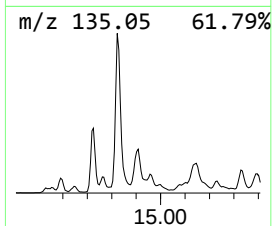
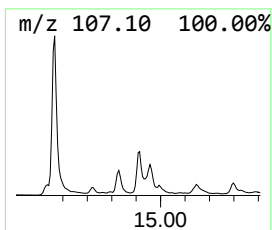
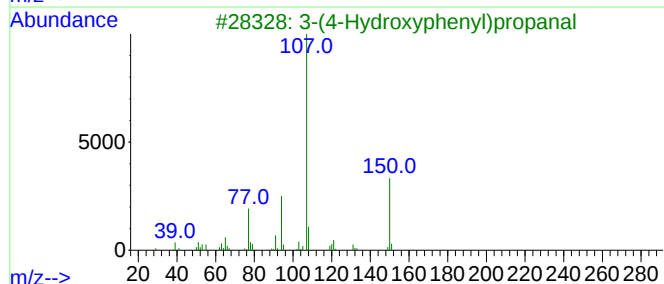
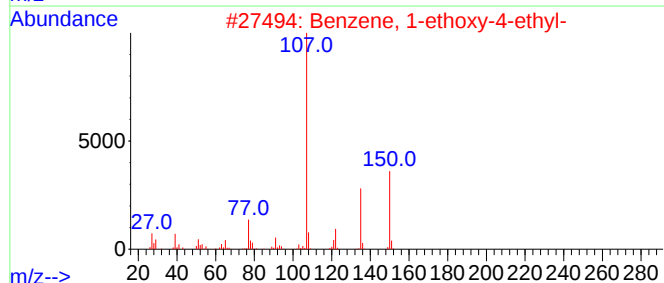
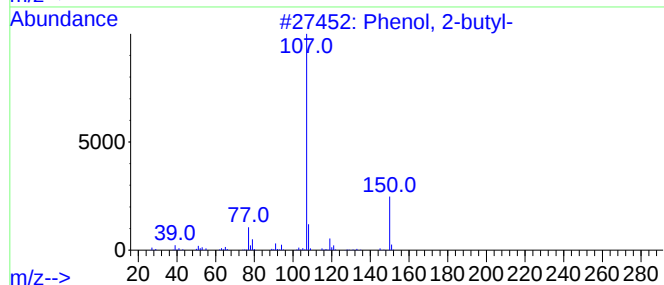
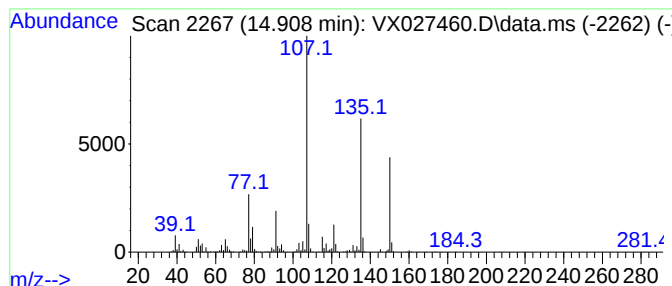
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Quant Title : SW846 8260

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

Peak Number 6 Phenol, 2-butyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.908	19.58 ug/l	561662	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 2-butyl-	150	C10H14O	003180-09-4	70
2			Benzene, 1-ethoxy-4-ethyl-	150	C10H14O	001585-06-4	64
3			3-(4-Hydroxyphenyl)propanal	150	C9H10O2	020238-83-9	58
4			Phenol, 4-(2-methylpropyl)-	150	C10H14O	004167-74-2	58
5			Urea, (3-methylphenyl)-	150	C8H10N2O	000063-99-0	52



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031522\
Data File : VX027460.D
Acq On : 15 Mar 2022 20:17
Operator : JC/MD
Sample : N1950-10
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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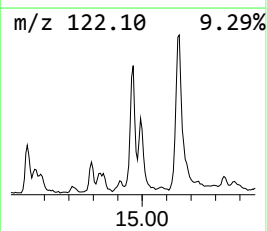
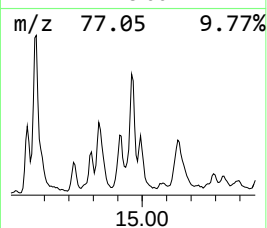
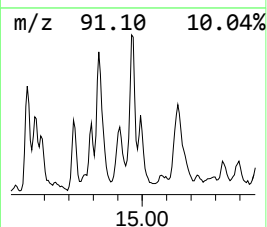
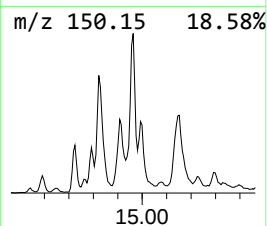
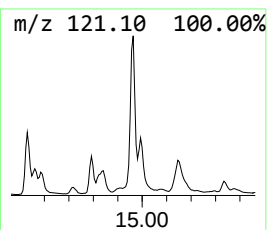
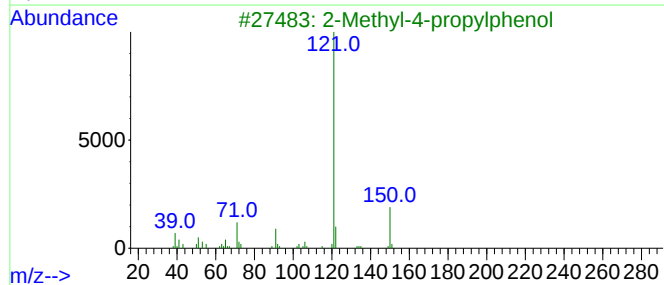
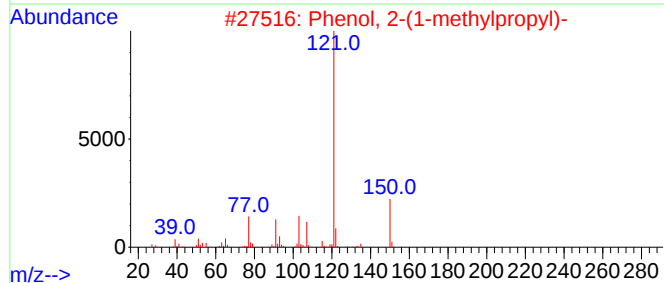
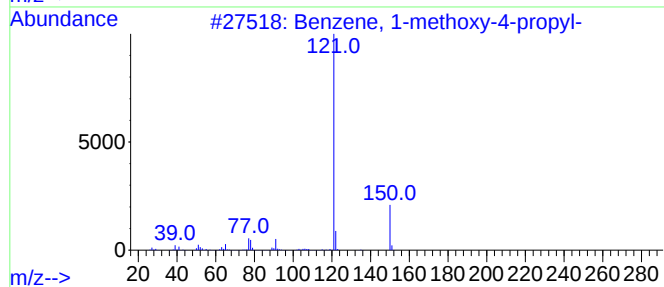
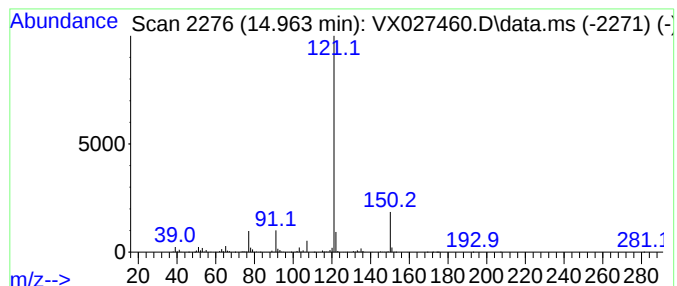
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, 1-methoxy-4-propyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.963	42.39 ug/l	1215900	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-methoxy-4-propyl-	150	C10H14O	000104-45-0	87
2			Phenol, 2-(1-methylpropyl)-	150	C10H14O	000089-72-5	86
3			2-Methyl-4-propylphenol	150	C10H14O	018441-56-0	80
4			Phenol, 4-(1-methylpropyl)-	150	C10H14O	000099-71-8	78
5			2-Methyl-6-propylphenol	150	C10H14O	003520-52-3	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031522\
Data File : VX027460.D
Acq On : 15 Mar 2022 20:17
Operator : JC/MD
Sample : N1950-10
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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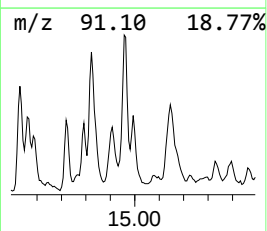
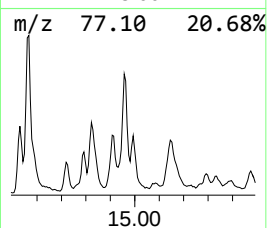
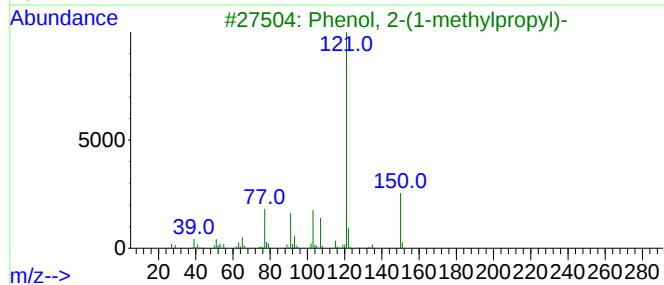
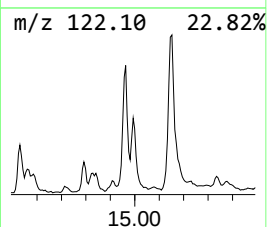
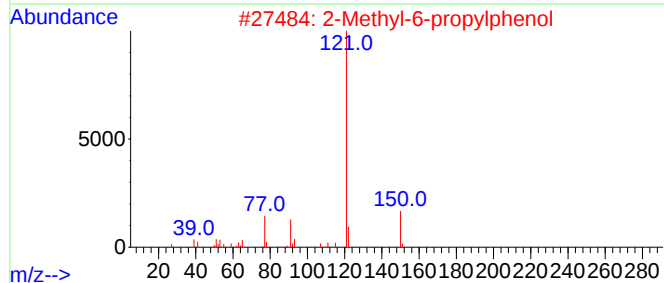
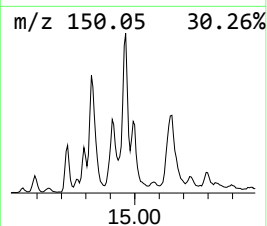
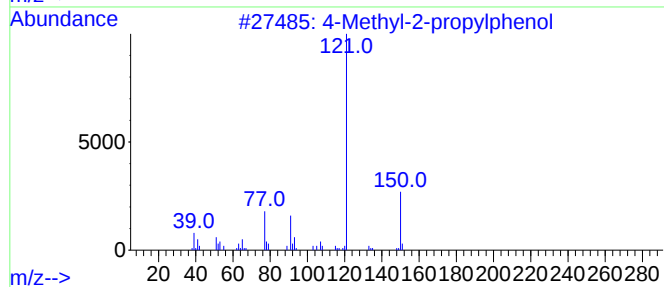
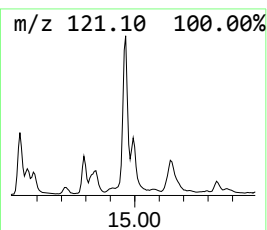
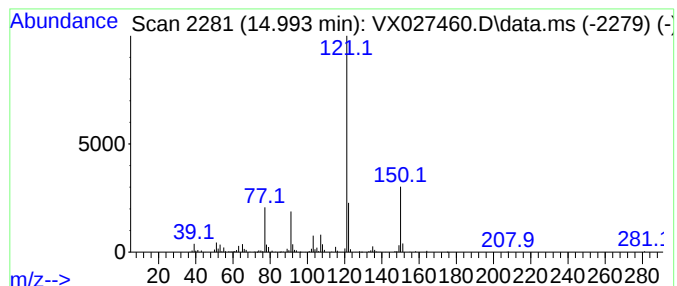
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Quant Title : SW846 8260

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

Peak Number 8 4-Methyl-2-propylphenol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.993	14.49 ug/l	415560	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Methyl-2-propylphenol	150	C10H14O	004074-46-8	80
2			2-Methyl-6-propylphenol	150	C10H14O	003520-52-3	72
3			Phenol, 2-(1-methylpropyl)-	150	C10H14O	000089-72-5	72
4			Fenobucarb	207	C12H17NO2	003766-81-2	64
5			2-sec-Butylphenol, acetate	192	C12H16O2	003056-61-9	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031522\
Data File : VX027460.D
Acq On : 15 Mar 2022 20:17
Operator : JC/MD
Sample : N1950-10
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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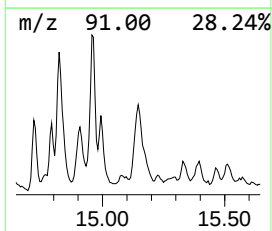
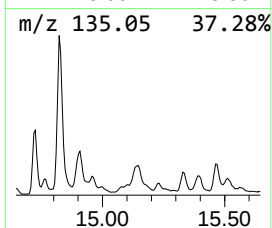
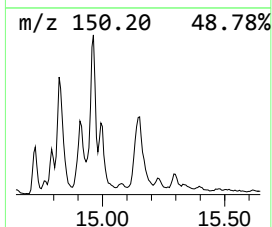
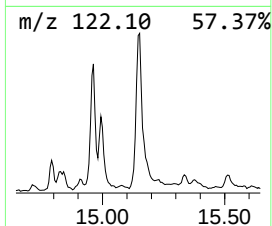
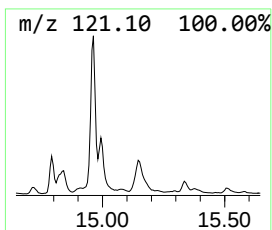
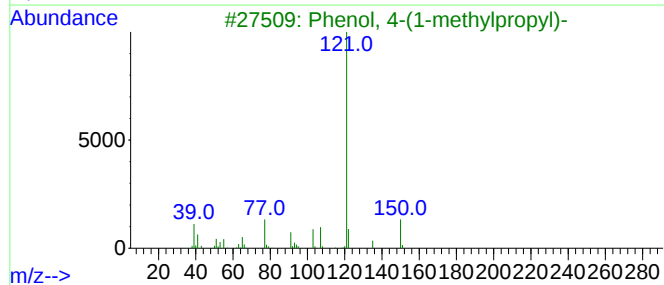
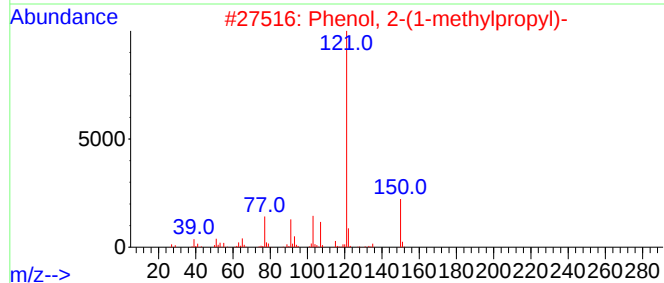
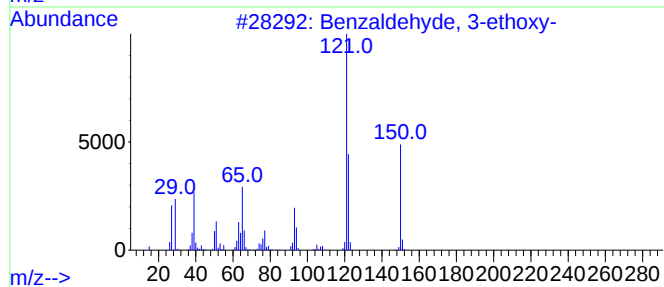
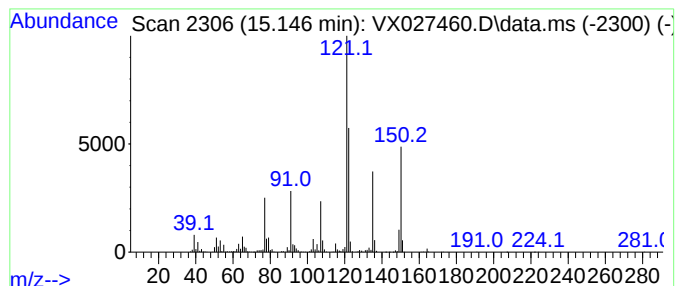
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Quant Title : SW846 8260

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

Peak Number 9 Benzaldehyde, 3-ethoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.146	29.65 ug/l	850553	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzaldehyde, 3-ethoxy-	150	C9H10O2	022924-15-8	53
2			Phenol, 2-(1-methylpropyl)-	150	C10H14O	000089-72-5	50
3			Phenol, 4-(1-methylpropyl)-	150	C10H14O	000099-71-8	50
4			Benzaldehyde, 4-ethoxy-	150	C9H10O2	010031-82-0	47
5			2-Methyl-6-propylphenol	150	C10H14O	003520-52-3	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031522\
Data File : VX027460.D
Acq On : 15 Mar 2022 20:17
Operator : JC/MD
Sample : N1950-10
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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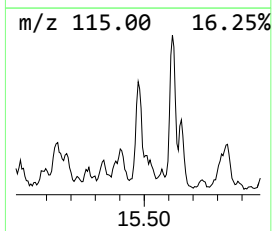
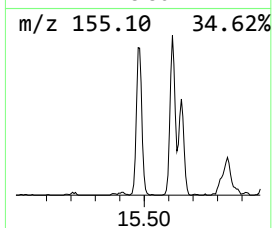
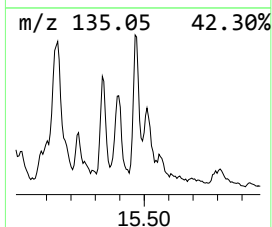
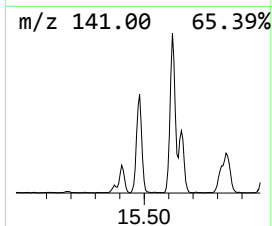
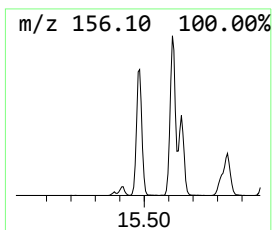
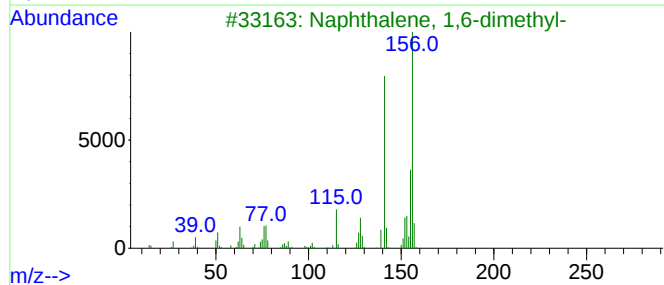
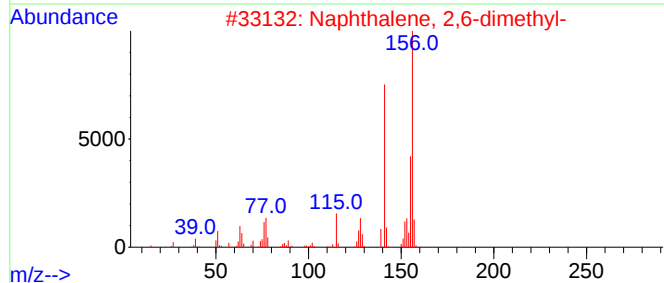
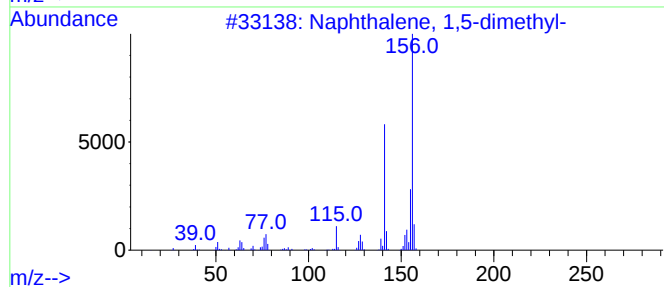
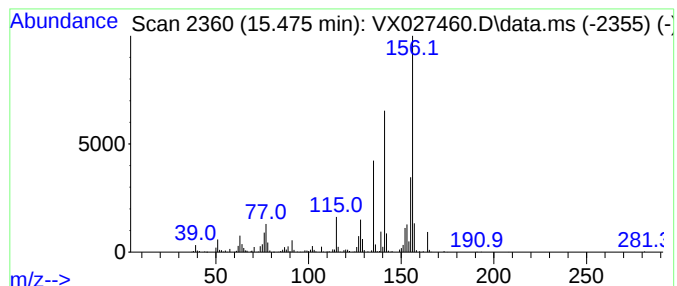
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Quant Title : SW846 8260

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

Peak Number 10 Naphthalene, 1,5-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.475	15.48 ug/l	444132	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	97
2			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	97
3			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	97
4			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	97
5			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	96



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031522\
Data File : VX027460.D
Acq On : 15 Mar 2022 20:17
Operator : JC/MD
Sample : N1950-10
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

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

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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Phenol, 3-ethyl...	14.530	18.9	ug/l	542002	4	12.024	1434170	50.0
Phenol, 4-propyl-	14.567	48.2	ug/l	1382700	4	12.024	1434170	50.0
Benzocyclohepta...	14.786	25.8	ug/l	738460	4	12.024	1434170	50.0
Phenol, 2-methy...	14.823	36.5	ug/l	1045800	4	12.024	1434170	50.0
Phenol, 2-butyl-	14.908	19.6	ug/l	561662	4	12.024	1434170	50.0
Benzene, 1-meth...	14.963	42.4	ug/l	1215900	4	12.024	1434170	50.0
4-Methyl-2-prop...	14.993	14.5	ug/l	415560	4	12.024	1434170	50.0
Benzaldehyde, 3...	15.146	29.6	ug/l	850553	4	12.024	1434170	50.0
Naphthalene, 1,...	15.475	15.5	ug/l	444132	4	12.024	1434170	50.0