

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX011921\
 Data File : VX020662.D
 Acq On : 19 Jan 2021 16:31
 Operator : JC/SP
 Sample : M1125-09 100X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 1714-1715

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\82X011921W.M

Title : SW846 8260

Signal : TIC: VX020662.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.099	159	166	177	rBV	38308	68954	2.50%	0.368%
2	2.416	211	218	234	rVB	574133	968777	35.11%	5.174%
3	3.008	306	315	325	rBV2	15723	42272	1.53%	0.226%
4	3.922	456	465	476	rBV2	9978	30762	1.11%	0.164%
5	5.458	706	717	729	rBV	150602	433980	15.73%	2.318%
6	5.623	729	744	764	rVB	243287	721344	26.14%	3.852%
7	5.897	779	789	800	rBV2	33086	90648	3.28%	0.484%
8	6.025	800	810	820	rBV	158552	417643	15.13%	2.230%
9	6.678	908	917	925	rBV	25010	58599	2.12%	0.313%
10	6.824	931	941	956	rBV	385612	911029	33.01%	4.865%
11	7.434	1031	1041	1050	rVB	11721	27685	1.00%	0.148%
12	8.696	1241	1248	1253	rBV	806669	1238741	44.89%	6.615%
13	8.763	1253	1259	1271	rVB	762854	1157219	41.93%	6.180%
14	10.092	1472	1477	1486	rVB	835646	1095327	39.69%	5.849%
15	10.232	1494	1500	1506	rBV	41403	54724	1.98%	0.292%
16	10.336	1506	1517	1523	rVV	115350	175837	6.37%	0.939%
17	10.683	1568	1574	1583	rVB	58713	81912	2.97%	0.437%
18	11.122	1640	1646	1656	rVB	666701	876652	31.77%	4.682%
19	11.415	1690	1694	1701	rBV	44741	83719	3.03%	0.447%
20	11.488	1701	1706	1708	rVV2	23980	40767	1.48%	0.218%
21	11.512	1708	1710	1716	rVB	41625	45878	1.66%	0.245%
22	11.652	1728	1733	1740	rVB	29287	43170	1.56%	0.231%
23	11.793	1752	1756	1765	rVB	77986	109176	3.96%	0.583%
24	12.061	1794	1800	1806	rBV	900070	1085448	39.33%	5.797%
25	12.128	1806	1811	1816	rVB2	30927	52656	1.91%	0.281%
26	12.280	1833	1836	1838	rBV2	25075	28367	1.03%	0.151%
27	12.354	1844	1848	1855	rVB3	37371	67390	2.44%	0.360%
28	12.457	1856	1865	1869	rBV	58127	75095	2.72%	0.401%
29	12.500	1869	1872	1879	rVB	19427	29069	1.05%	0.155%
30	12.738	1905	1911	1914	rBV2	17653	32390	1.17%	0.173%
31	13.000	1951	1954	1961	rVB3	22251	45014	1.63%	0.240%
32	13.207	1980	1988	1992	rBV3	24605	42499	1.54%	0.227%
33	13.305	1998	2004	2006	rBV	56546	77836	2.82%	0.416%
34	13.329	2006	2008	2013	rVB3	68280	85253	3.09%	0.455%
35	13.457	2025	2029	2038	rVB	62812	108132	3.92%	0.577%
36	13.622	2053	2056	2061	rBV4	18445	31675	1.15%	0.169%

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37	13.713	2067	2071	2077	rBV5	18801	36581	1.33%	0.195%
38	13.817	2083	2088	2094	rBV	1437437	1795771	65.07%	9.590%
39	13.884	2094	2099	2106	rVB4	37043	81302	2.95%	0.434%
40	13.963	2106	2112	2117	rBV3	50717	88840	3.22%	0.474%
41	14.073	2127	2130	2133	rBV	54404	59219	2.15%	0.316%
42	14.115	2133	2137	2141	rBV	95358	119584	4.33%	0.639%
43	14.256	2156	2160	2167	rVB3	111275	208237	7.55%	1.112%
44	14.359	2172	2177	2181	rBV	128840	172267	6.24%	0.920%
45	14.408	2182	2185	2189	rVB	61369	72691	2.63%	0.388%
46	14.518	2199	2203	2212	rBV5	45767	106855	3.87%	0.571%
47	14.597	2213	2216	2222	rBV6	24612	46446	1.68%	0.248%
48	14.676	2222	2229	2234	rBV	2225855	2759569	100.00%	14.737%
49	14.816	2245	2252	2257	rBV	1121235	1502506	54.45%	8.024%
50	15.140	2302	2305	2309	rBV3	35248	55387	2.01%	0.296%
51	15.225	2315	2319	2321	rBV2	69612	105763	3.83%	0.565%
52	15.255	2321	2324	2328	rVB2	115209	143749	5.21%	0.768%
53	15.420	2348	2351	2354	rBV	59743	73182	2.65%	0.391%
54	15.530	2364	2369	2376	rBV2	162602	329438	11.94%	1.759%
55	15.664	2387	2391	2395	rBV	172784	240639	8.72%	1.285%
56	16.146	2466	2470	2477	rBV2	91544	191824	6.95%	1.024%

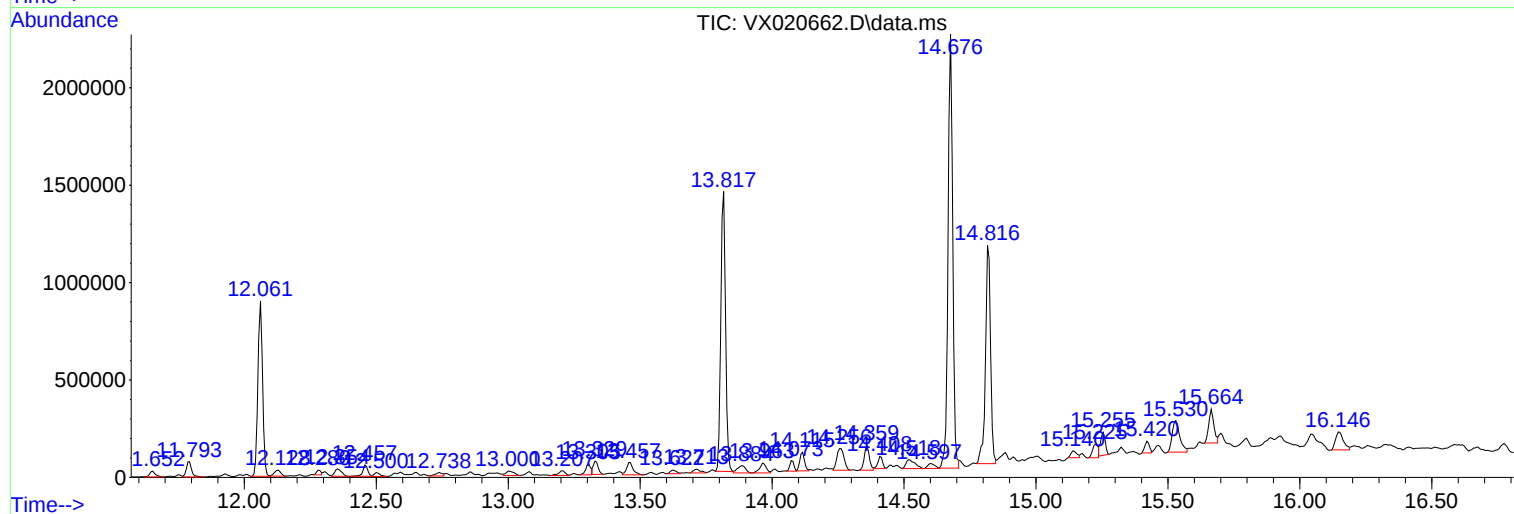
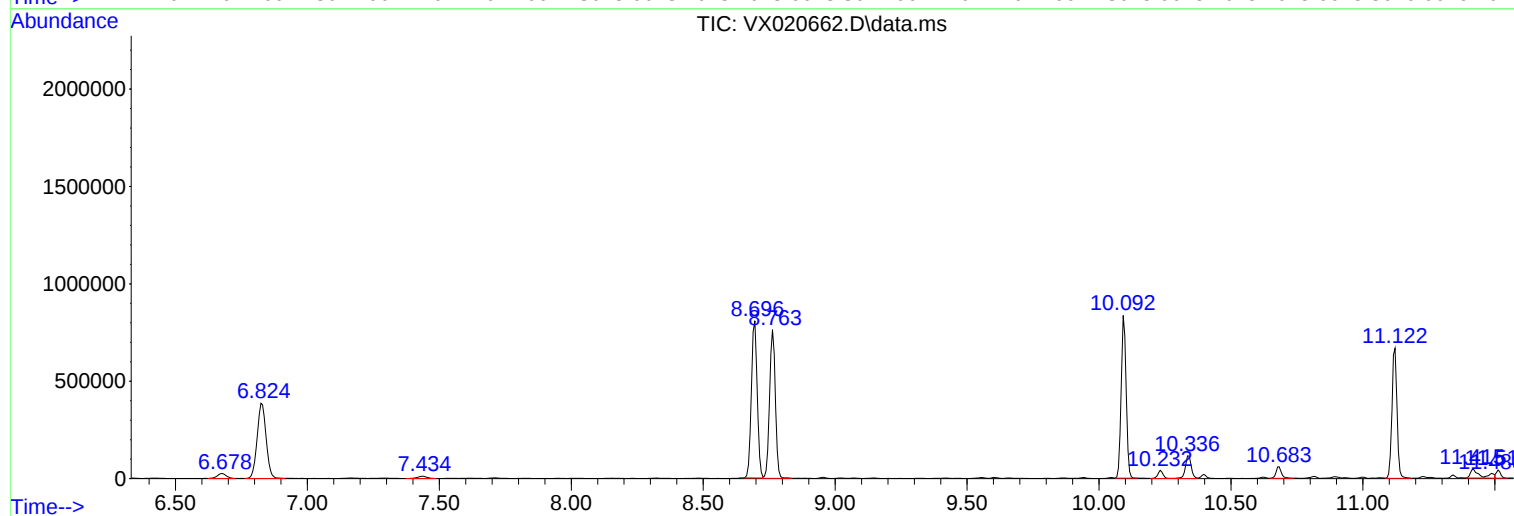
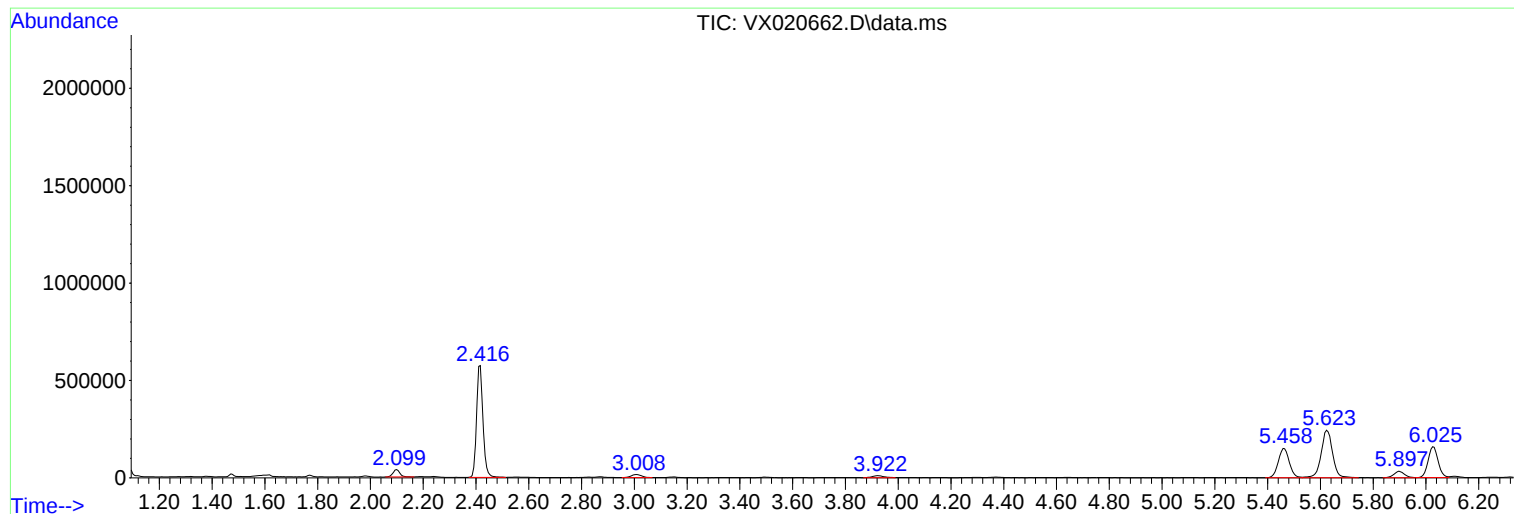
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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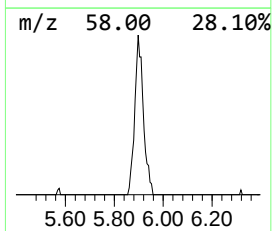
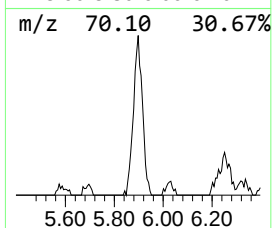
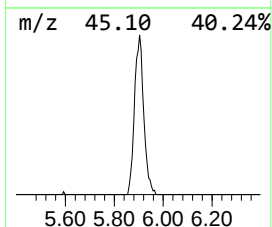
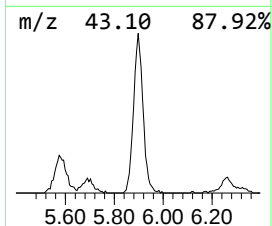
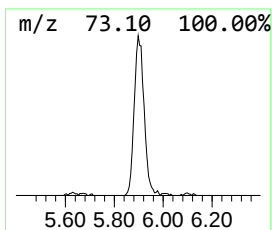
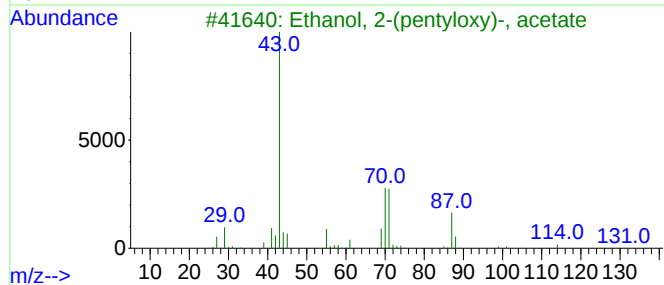
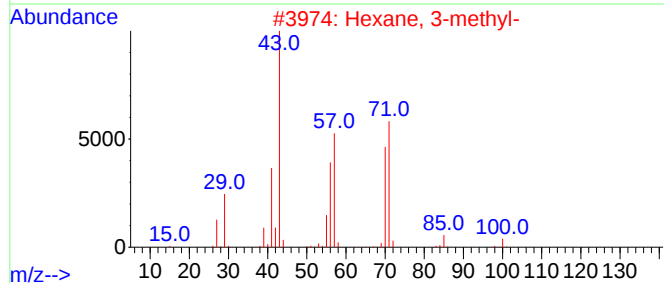
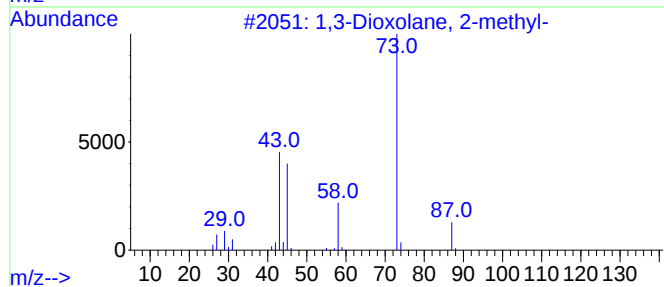
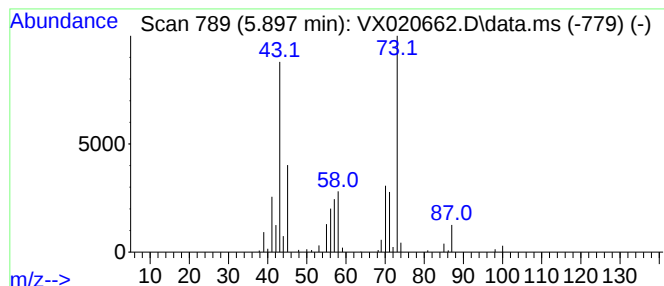
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X011921W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown5.897 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.897	6.28 ug/l	90648	Pentafluorobenzene	5.623

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	43
2			Hexane, 3-methyl-	100	C7H16	000589-34-4	30
3			Ethanol, 2-(pentyloxy)-, acetate	174	C9H18O3	005312-09-4	27
4			2-Heptanone, 5-methyl-	128	C8H16O	018217-12-4	25
5			Hydroperoxide, 1-methylethyl	76	C3H8O2	003031-75-2	25



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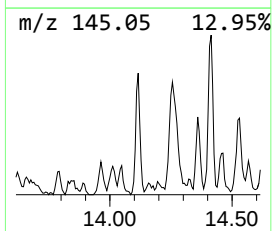
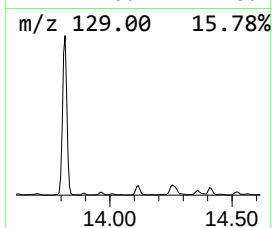
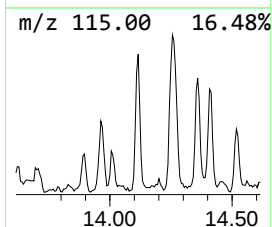
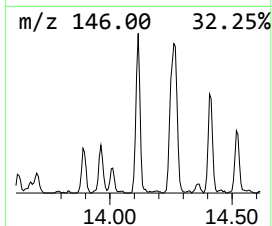
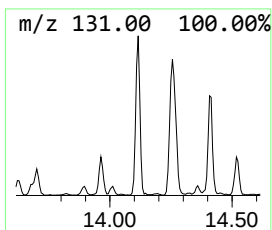
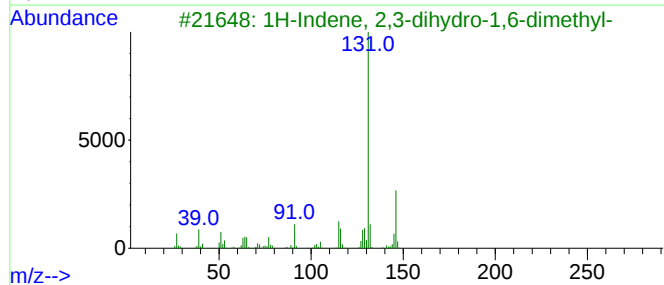
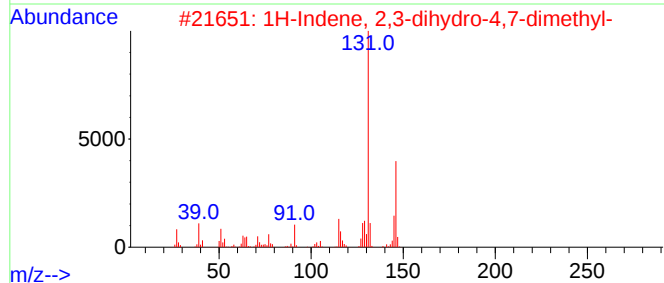
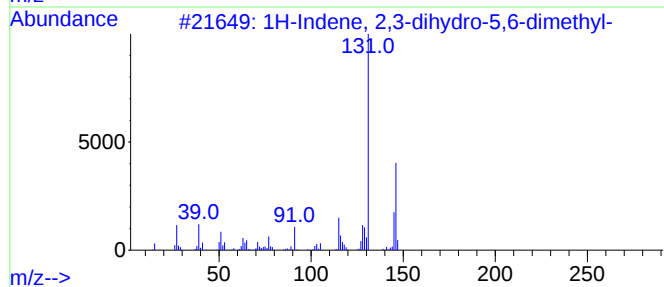
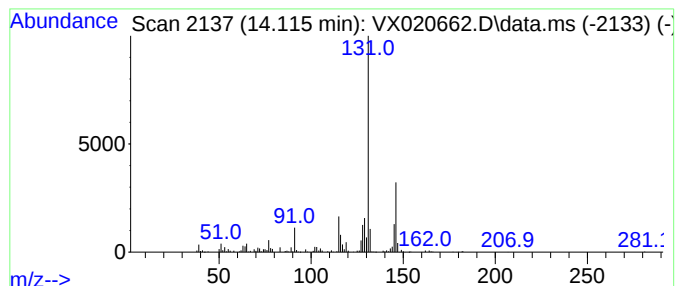
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 1H-Indene, 2,3-dihydro-5,6-... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.115	5.51 ug/l	119584	1,4-Dichlorobenzene-d4	12.061

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Indene, 2,3-dihydro-5,6-dimet...	146	C11H14	001075-22-5	96
2			1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	94
3			1H-Indene, 2,3-dihydro-1,6-dimet...	146	C11H14	017059-48-2	93
4			Benzene, (1,2-dimethyl-1-propenyl)-	146	C11H14	000769-57-3	91
5			Benzene, 1-methyl-4-(1-methyl-2-...	146	C11H14	097664-18-1	91



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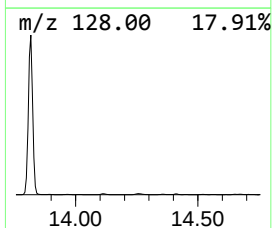
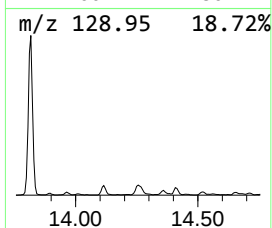
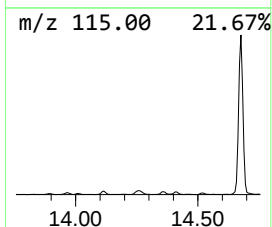
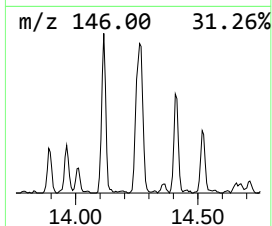
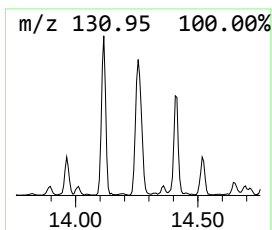
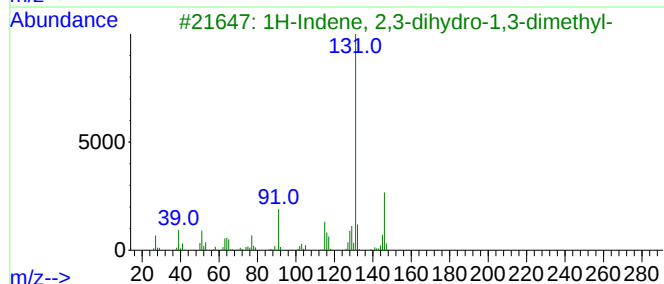
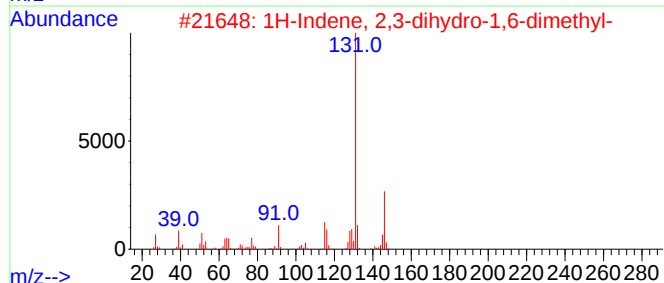
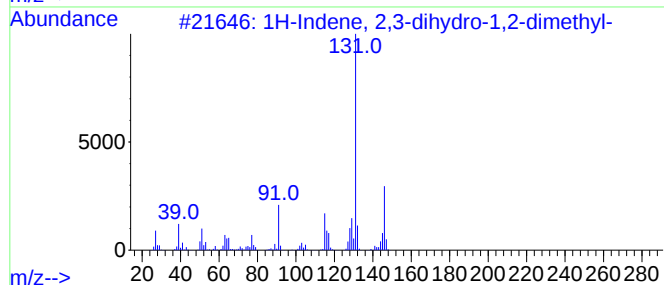
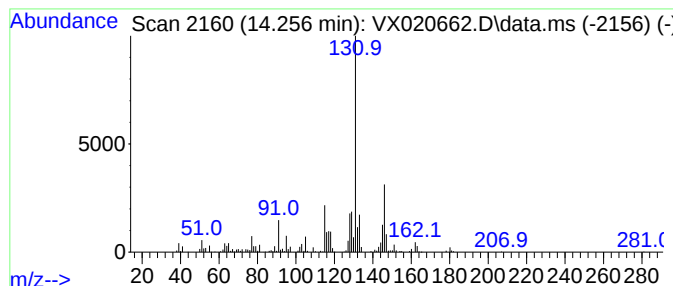
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 1H-Indene, 2,3-dihydro-1,2-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.256	9.59 ug/l	208237	1,4-Dichlorobenzene-d4	12.061

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	91
2			1H-Indene, 2,3-dihydro-1,6-dimet...	146	C11H14	017059-48-2	87
3			1H-Indene, 2,3-dihydro-1,3-dimet...	146	C11H14	004175-53-5	83
4			Benzene, (1,2-dimethyl-1-propenyl)-	146	C11H14	000769-57-3	81
5			1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	81



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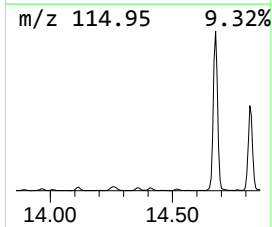
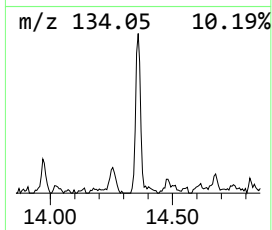
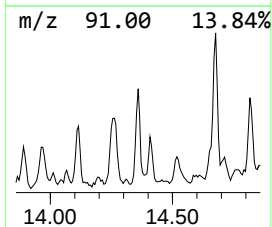
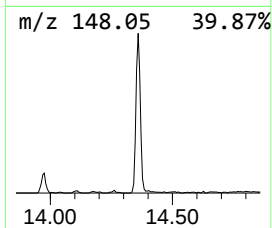
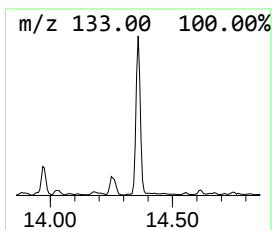
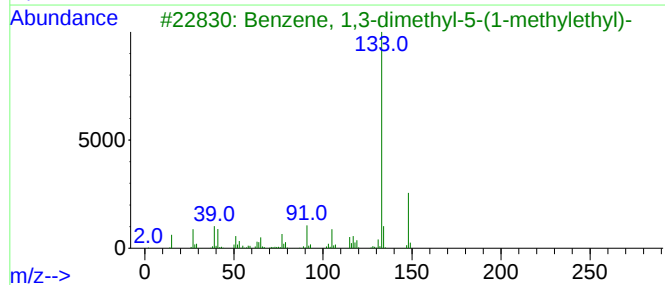
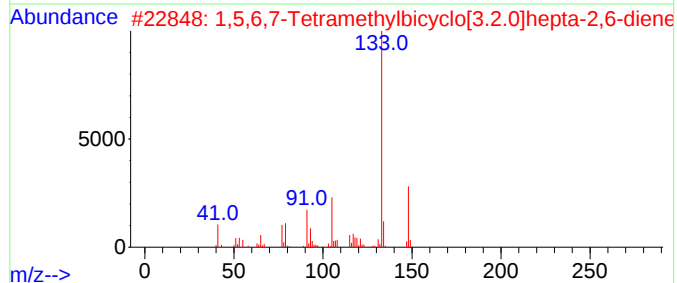
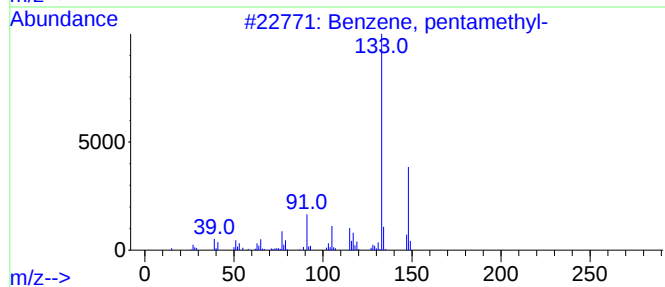
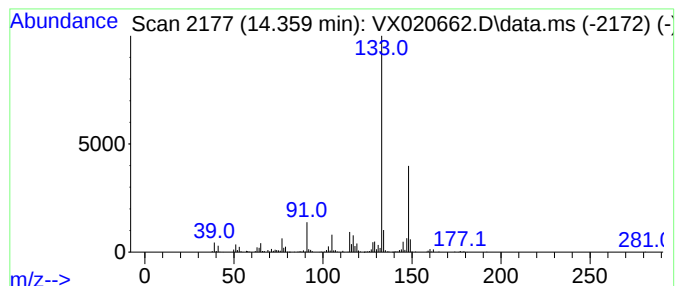
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzene, pentamethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.359	7.94 ug/l	172267	1,4-Dichlorobenzene-d4	12.061

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, pentamethyl-	148	C11H16	000700-12-9	93
2			1,5,6,7-Tetramethylbicyclo[3.2.0]hepta-2,6-diene	148	C11H16	134329-46-7	90
3			Benzene, 1,3-dimethyl-5-(1-methylethyl)-	148	C11H16	004706-90-5	87
4			Benzene, 2,4-dimethyl-1-(1-methylethyl)-	148	C11H16	004706-89-2	87
5			3,4-Dimethylcumene	148	C11H16	1000370-34-1	87



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MSVOA_X
ClientSampleId :
1714-1715

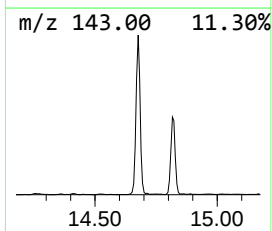
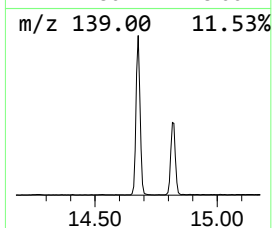
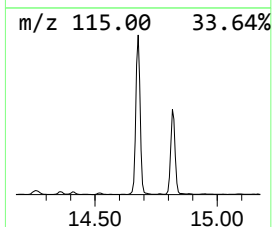
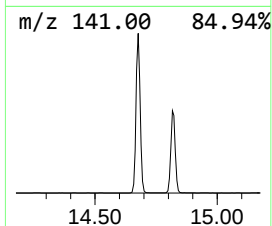
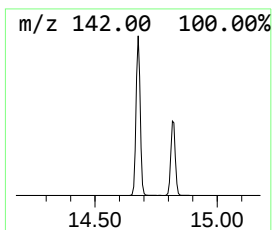
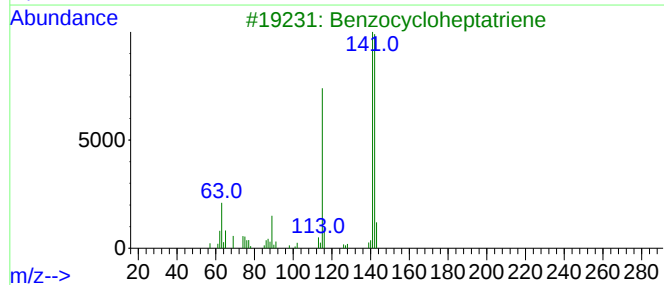
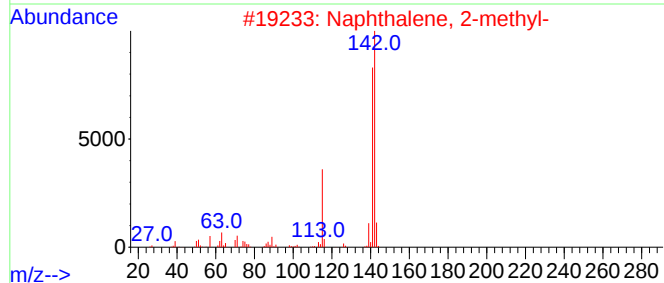
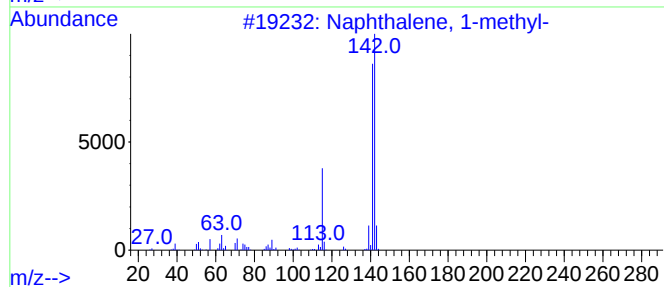
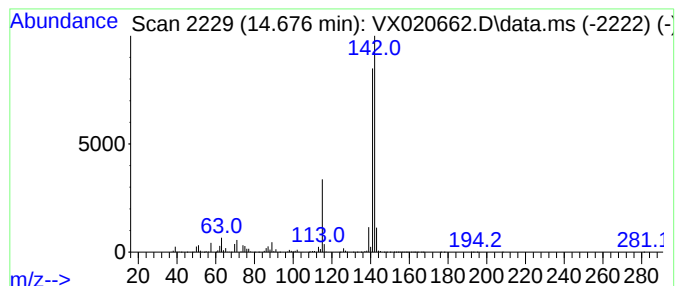
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Naphthalene, 1-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.676	127.12 ug/l	2759570	1,4-Dichlorobenzene-d4	12.061

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
2			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
3			Benzocycloheptatriene	142	C11H10	000264-09-5	91
4			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
5			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX011921\
Data File : VX020662.D
Acq On : 19 Jan 2021 16:31
Operator : JC/SP
Sample : M1125-09 100X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1714-1715

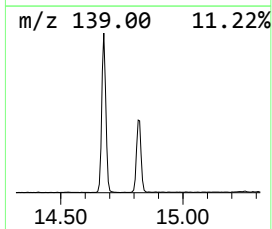
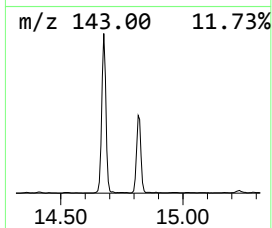
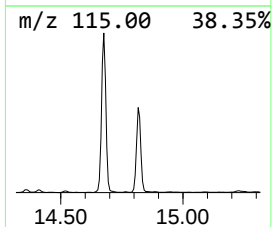
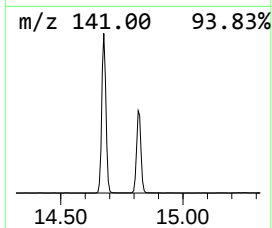
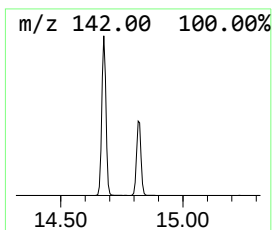
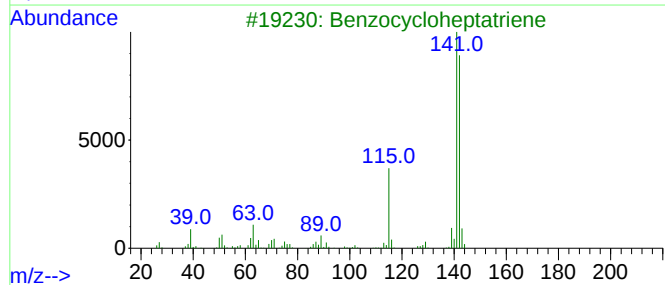
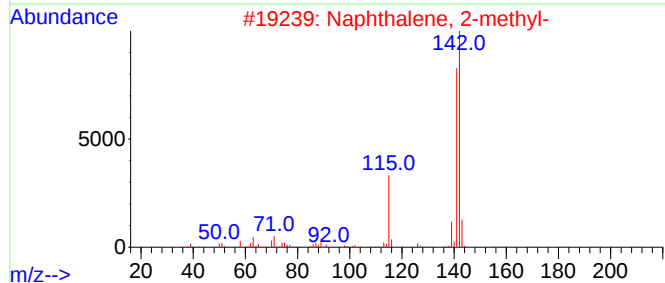
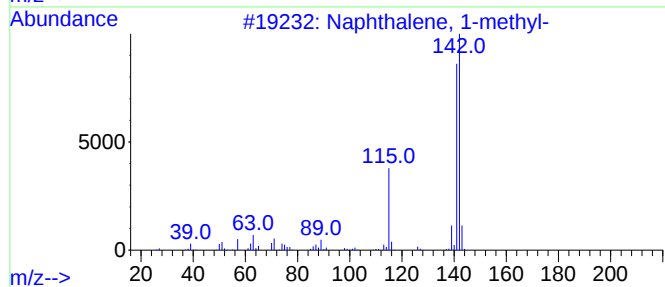
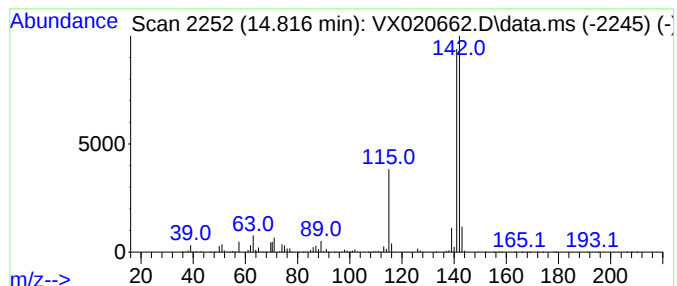
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Naphthalene, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.817	69.21 ug/l	1502510	1,4-Dichlorobenzene-d4	12.061

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
2			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
3			Benzocycloheptatriene	142	C11H10	000264-09-5	91
4			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	90
5			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX011921\
Data File : VX020662.D
Acq On : 19 Jan 2021 16:31
Operator : JC/SP
Sample : M1125-09 100X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1714-1715

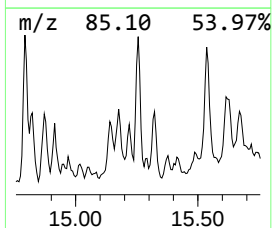
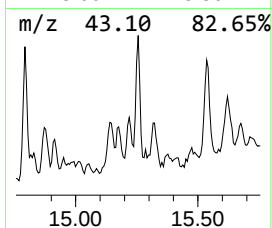
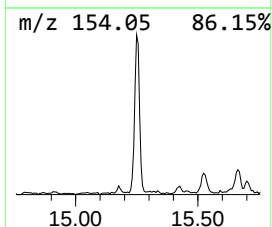
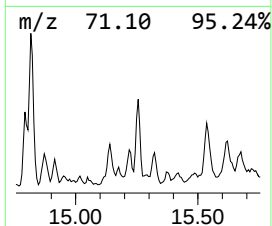
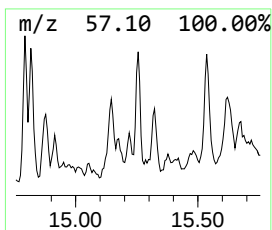
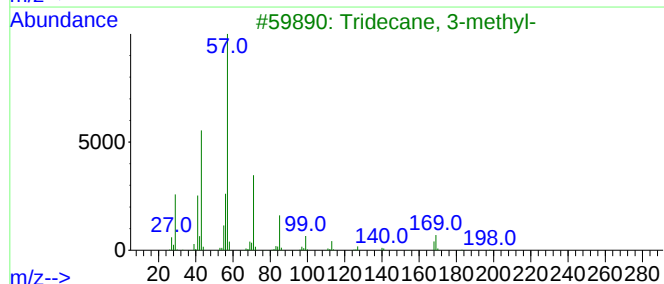
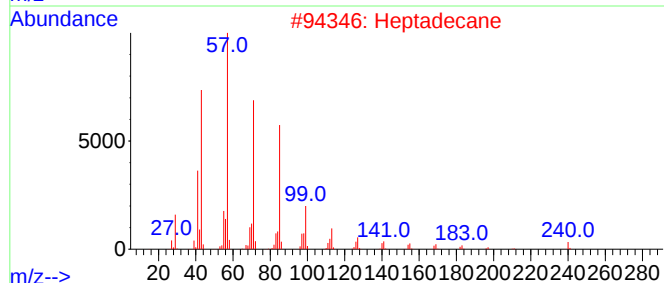
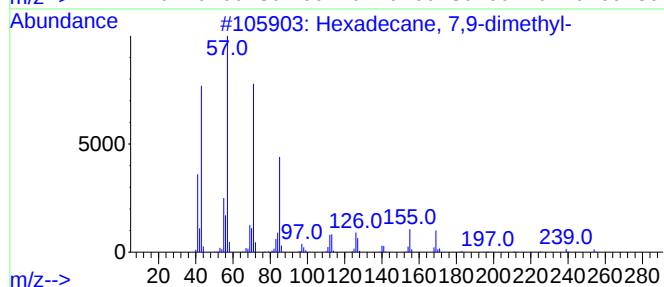
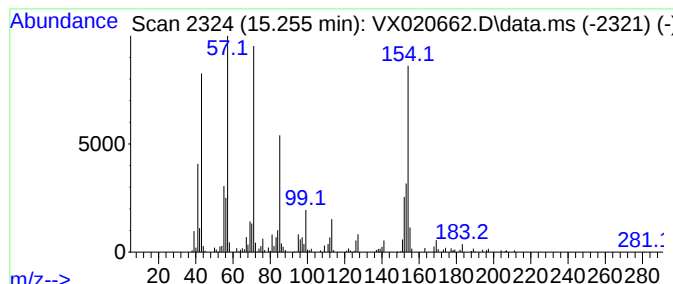
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 unknown15.255 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.255	6.62 ug/l	143749	1,4-Dichlorobenzene-d4	12.061

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane, 7,9-dimethyl-	254	C18H38	021164-95-4	49
2			Heptadecane	240	C17H36	000629-78-7	49
3			Tridecane, 3-methyl-	198	C14H30	006418-41-3	45
4			Decane, 3,6-dimethyl-	170	C12H26	017312-53-7	45
5			Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	45



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX011921\
Data File : VX020662.D
Acq On : 19 Jan 2021 16:31
Operator : JC/SP
Sample : M1125-09 100X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1714-1715

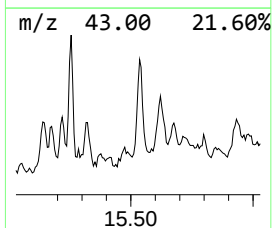
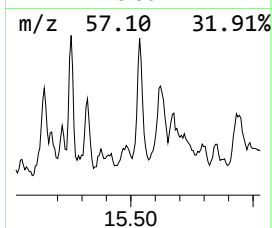
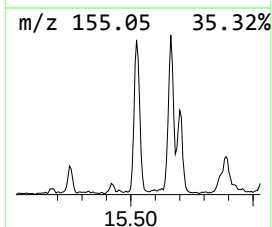
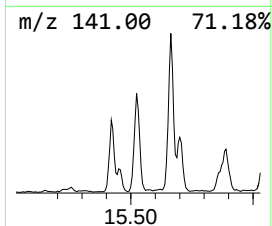
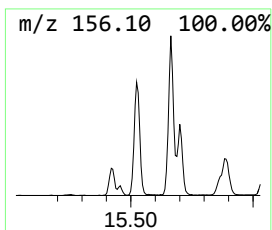
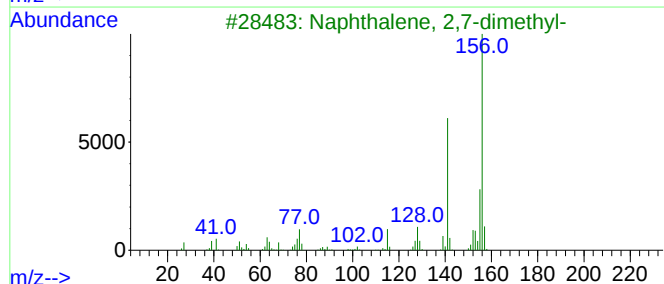
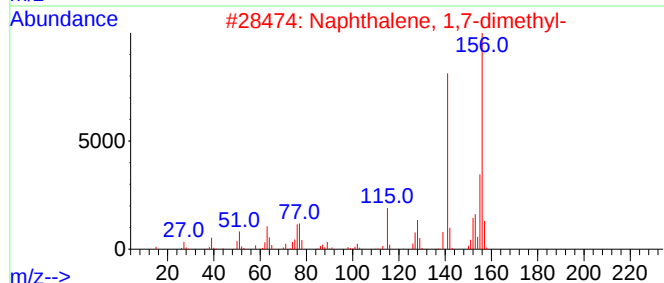
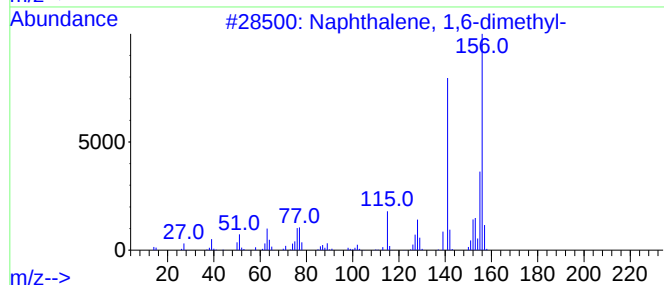
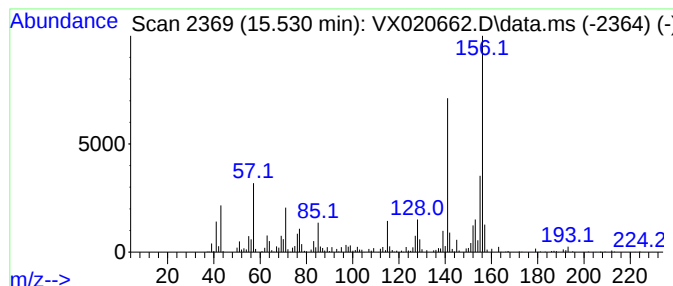
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Naphthalene, 1,6-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.530	15.18 ug/l	329438	1,4-Dichlorobenzene-d4	12.061

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	97
2			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	96
3			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	96
4			Naphthalene, 1,2-dimethyl-	156	C12H12	000573-98-8	96
5			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	96



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX011921\
Data File : VX020662.D
Acq On : 19 Jan 2021 16:31
Operator : JC/SP
Sample : M1125-09 100X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1714-1715

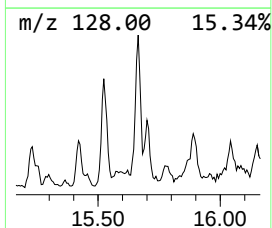
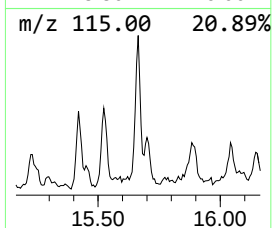
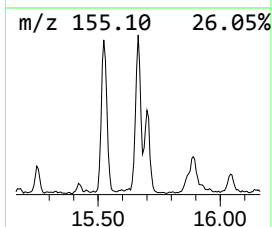
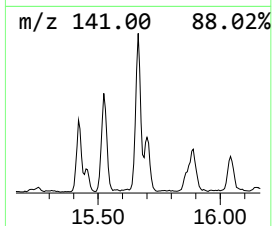
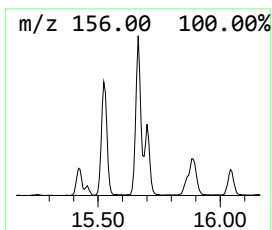
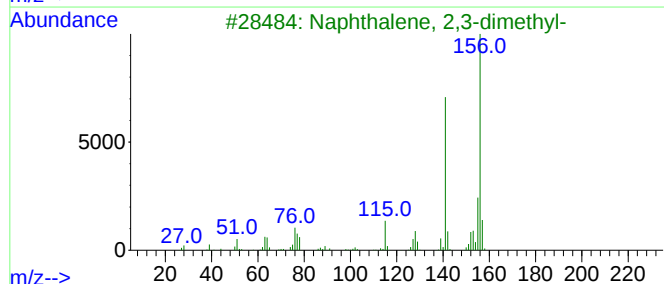
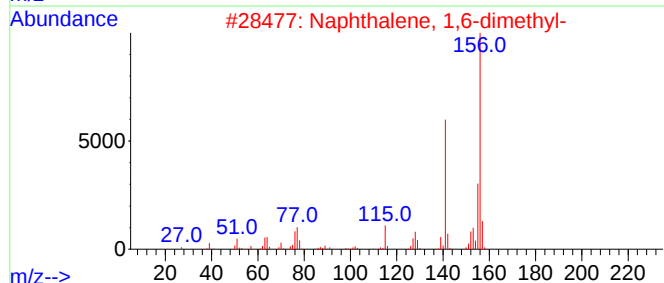
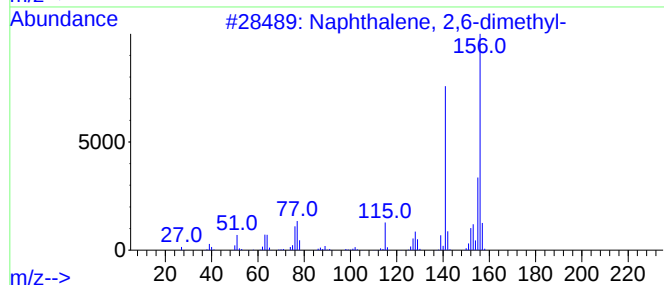
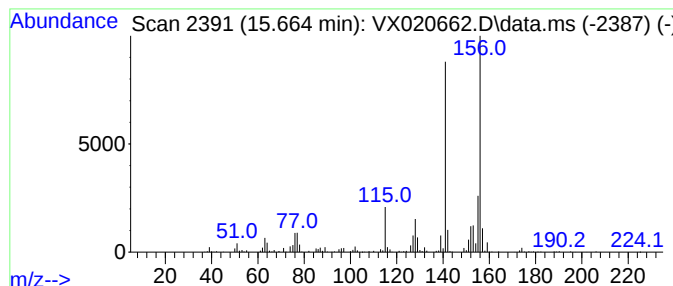
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X011921W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Naphthalene, 2,6-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.664	11.08 ug/l	240639	1,4-Dichlorobenzene-d4	12.061

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	97
2			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	97
3			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	97
4			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	97
5			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	97



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX011921\
Data File : VX020662.D
Acq On : 19 Jan 2021 16:31
Operator : JC/SP
Sample : M1125-09 100X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1714-1715

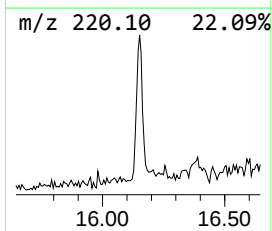
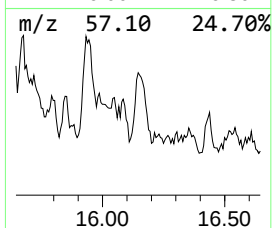
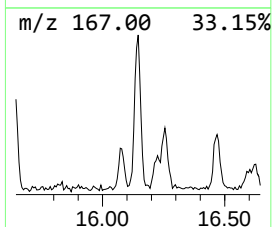
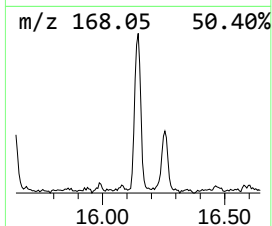
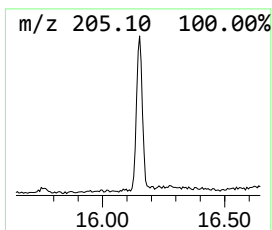
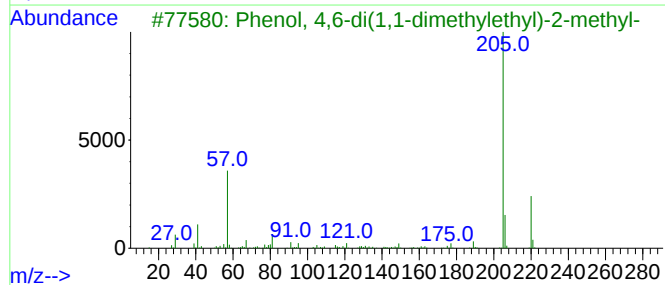
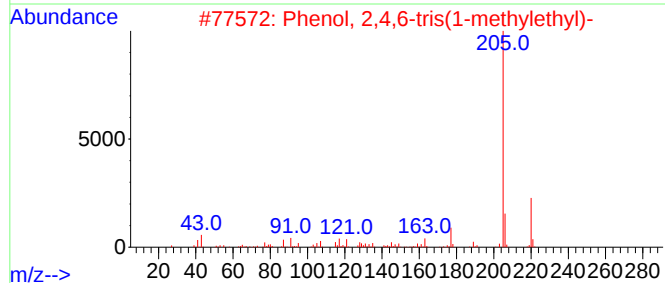
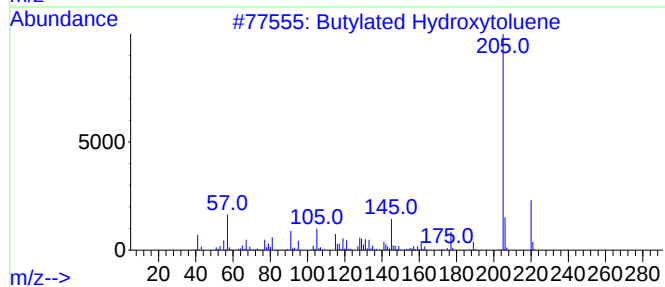
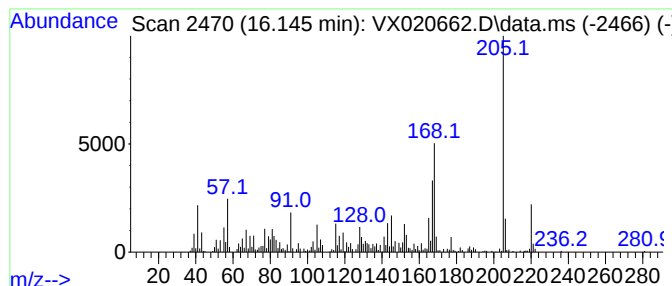
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Butylated Hydroxytoluene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.145	8.84 ug/l	191824	1,4-Dichlorobenzene-d4	12.061

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	78
2			Phenol, 2,4,6-tris(1-methylethyl)-	220	C15H24O	002934-07-8	45
3			Phenol, 4,6-di(1,1-dimethylethyl)-	220	C15H24O	000616-55-7	45
4			4,6-di-tert-Butyl-m-cresol	220	C15H24O	000497-39-2	43
5			1,1'-Biphenyl, 3-methyl-	168	C13H12	000643-93-6	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX011921\
Data File : VX020662.D
Acq On : 19 Jan 2021 16:31
Operator : JC/SP
Sample : M1125-09 100X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1714-1715

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X011921W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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1H-Indene, 2,3-...	14.115	5.5	ug/l	119584	4	12.061	1085450	50.0
1H-Indene, 2,3-...	14.256	9.6	ug/l	208237	4	12.061	1085450	50.0
Benzene, pentam...	14.359	7.9	ug/l	172267	4	12.061	1085450	50.0
Naphthalene, 1-...	14.676	127.1	ug/l	2759570	4	12.061	1085450	50.0
Naphthalene, 2-...	14.817	69.2	ug/l	1502510	4	12.061	1085450	50.0
unknown15.255	15.255	6.6	ug/l	143749	4	12.061	1085450	50.0
Naphthalene, 1,...	15.530	15.2	ug/l	329438	4	12.061	1085450	50.0
Naphthalene, 2,...	15.664	11.1	ug/l	240639	4	12.061	1085450	50.0
Butylated Hydro...	16.145	8.8	ug/l	191824	4	12.061	1085450	50.0