

Data Path : W:\HPCHEM1\MSVOA X\DATA\VX052518\
 Data File : VX001980.D
 Acq On : 25 May 2018 16:36
 Operator : JC/MD
 Sample : J3015-15
 Misc : 5.48g/5mL/100uL/5mL/MSVOA_X/MEOH
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 AOC7-BTM-5-5.5

Integration Parameters: RTEINT.P

Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : W:\HPCHEM1\MSVOA_X\METHOD\82X052418W.M
 Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.069	75	79	93	rBV	1372113	1606956	52.33%	2.683%
2	1.642	156	173	174	rBV7	41025	162281	5.28%	0.271%
3	3.026	395	400	410	rVB	21832	50243	1.64%	0.084%
4	5.513	795	808	821	rBV	256796	761065	24.78%	1.271%
5	5.659	822	832	849	rVB	304883	861192	28.05%	1.438%
6	6.074	889	900	916	rBV	289587	763269	24.86%	1.274%
7	6.860	1019	1029	1047	rBV	449843	1102718	35.91%	1.841%
8	8.720	1327	1334	1349	rVB	1345346	2174949	70.83%	3.632%
9	8.976	1370	1376	1383	rBV2	31421	53485	1.74%	0.089%
10	9.561	1467	1472	1479	rBV2	33060	65593	2.14%	0.110%
11	9.878	1520	1524	1528	rBV3	19512	40410	1.32%	0.067%
12	9.964	1534	1538	1544	rVB	130140	184346	6.00%	0.308%
13	10.067	1549	1555	1559	rBV	114637	159205	5.18%	0.266%
14	10.122	1559	1564	1573	rVV	970979	1377161	44.85%	2.299%
15	10.256	1581	1586	1591	rVB	63796	89911	2.93%	0.150%
16	10.366	1591	1604	1609	rVV2	118987	227406	7.41%	0.380%
17	10.421	1609	1613	1624	rVB	178144	271518	8.84%	0.453%
18	10.646	1645	1650	1653	rBV	85250	109273	3.56%	0.182%
19	10.707	1653	1660	1662	rBV	140572	201282	6.55%	0.336%
20	10.774	1668	1671	1674	rVB	36994	46405	1.51%	0.077%
21	10.841	1674	1682	1685	rBV	117754	198907	6.48%	0.332%
22	10.915	1685	1694	1698	rBV3	88024	165674	5.40%	0.277%
23	10.957	1698	1701	1705	rVB2	32808	44021	1.43%	0.074%
24	11.024	1705	1712	1716	rBV	83105	134664	4.39%	0.225%
25	11.085	1718	1722	1726	rBV	116391	160365	5.22%	0.268%
26	11.146	1726	1732	1742	rVB2	1515448	2344789	76.36%	3.915%
27	11.250	1745	1749	1753	rVB	250035	283044	9.22%	0.473%
28	11.366	1764	1768	1776	rBV	195243	248362	8.09%	0.415%
29	11.439	1776	1780	1782	rBV	346436	462452	15.06%	0.772%
30	11.512	1787	1792	1794	rBV	622169	814134	26.51%	1.359%
31	11.536	1794	1796	1803	rVB	527734	580872	18.92%	0.970%
32	11.677	1814	1819	1826	rBV	434203	675512	22.00%	1.128%
33	11.744	1826	1830	1832	rBV	86890	102523	3.34%	0.171%
34	11.774	1832	1835	1837	rBV	118952	116886	3.81%	0.195%

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35	11.811	1837	1841	1850	rVB	2316641	3070671	100.00%	5.127%
36	11.896	1851	1855	1858	rBV	122231	178793	5.82%	0.299%
37	11.927	1858	1860	1861	rBV	47274	41015	1.34%	0.068%
38	11.951	1861	1864	1868	rVB2	142293	180064	5.86%	0.301%
39	12.000	1868	1872	1874	rBV3	91323	143717	4.68%	0.240%
40	12.030	1874	1877	1880	rVB	195034	206452	6.72%	0.345%
41	12.085	1880	1886	1891	rBV2	1388907	1939653	63.17%	3.239%
42	12.152	1891	1897	1902	rBV3	705449	1142666	37.21%	1.908%
43	12.231	1907	1910	1916	rVB2	269097	318798	10.38%	0.532%
44	12.311	1917	1923	1924	rBV	736919	986865	32.14%	1.648%
45	12.329	1924	1926	1930	rVB	1086655	1110764	36.17%	1.855%
46	12.378	1930	1934	1941	rVB3	1846565	2803667	91.30%	4.681%
47	12.439	1941	1944	1945	rBV3	44360	48717	1.59%	0.081%
48	12.481	1945	1951	1955	rBV2	647038	776597	25.29%	1.297%
49	12.524	1955	1958	1964	rVB	505757	631459	20.56%	1.054%
50	12.591	1964	1969	1971	rBV	924289	1170655	38.12%	1.955%
51	12.615	1971	1973	1979	rVB	855563	901579	29.36%	1.505%
52	12.676	1979	1983	1986	rBV	1476678	1672032	54.45%	2.792%
53	12.707	1986	1988	1992	rVB	173019	175052	5.70%	0.292%
54	12.762	1992	1997	2006	rVB3	526151	1260503	41.05%	2.105%
55	12.859	2007	2013	2018	rBV4	156421	289353	9.42%	0.483%
56	12.908	2018	2021	2025	rVB	355416	414801	13.51%	0.693%
57	12.981	2025	2033	2037	rBV	997460	1600010	52.11%	2.672%
58	13.024	2037	2040	2046	rVB	1526138	1827752	59.52%	3.052%
59	13.085	2046	2050	2051	rBV	433162	482736	15.72%	0.806%
60	13.103	2051	2053	2056	rVV2	342602	408543	13.30%	0.682%
61	13.134	2056	2058	2061	rVB	415060	377267	12.29%	0.630%
62	13.176	2061	2065	2068	rBV2	297593	348319	11.34%	0.582%
63	13.225	2068	2073	2078	rVB2	861053	1420630	46.26%	2.372%
64	13.274	2078	2081	2084	rBV2	419880	484747	15.79%	0.809%
65	13.323	2084	2089	2091	rBV5	615952	896752	29.20%	1.497%
66	13.359	2091	2095	2099	rVB3	1646461	2179411	70.98%	3.639%
67	13.432	2104	2107	2112	rVV	569857	842613	27.44%	1.407%
68	13.487	2112	2116	2124	rVB5	265538	525664	17.12%	0.878%
69	13.567	2124	2129	2132	rBV2	285583	451472	14.70%	0.754%
70	13.609	2132	2136	2138	rVV	439758	662364	21.57%	1.106%
71	13.640	2138	2141	2149	rVV3	726943	1551012	50.51%	2.590%

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ClientSampleId :
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72	13.737	2152	2157	2161	rVV3	459310	879635	28.65%	1.469%
73	13.780	2161	2164	2170	rVV4	178186	366057	11.92%	0.611%
74	13.841	2170	2174	2179	rVV	584819	836439	27.24%	1.397%
75	13.890	2179	2182	2184	rVV3	122397	169609	5.52%	0.283%
76	13.920	2185	2187	2192	rVB3	173101	231656	7.54%	0.387%
77	13.993	2192	2199	2203	rBV4	328517	658156	21.43%	1.099%
78	14.036	2203	2206	2209	rVV2	164968	206082	6.71%	0.344%
79	14.097	2213	2216	2219	rVB3	265725	295669	9.63%	0.494%
80	14.140	2219	2223	2227	rBV2	427383	515098	16.77%	0.860%
81	14.225	2234	2237	2241	rVB	93525	109642	3.57%	0.183%
82	14.280	2241	2246	2255	rVB	415634	646652	21.06%	1.080%
83	14.383	2259	2263	2268	rBV	208717	278981	9.09%	0.466%
84	14.438	2268	2272	2276	rVB	234846	267028	8.70%	0.446%
85	14.481	2276	2279	2285	rVB7	55841	99794	3.25%	0.167%
86	14.548	2285	2290	2295	rBV4	81930	185377	6.04%	0.310%
87	14.700	2307	2315	2320	rBV	1180465	1591886	51.84%	2.658%
88	14.792	2325	2330	2331	rBV2	55563	67088	2.18%	0.112%
89	14.816	2331	2334	2336	rVV	118299	145689	4.74%	0.243%
90	14.847	2336	2339	2343	rVV	588416	706623	23.01%	1.180%
91	15.255	2402	2406	2409	rBV	60267	100293	3.27%	0.167%
92	15.450	2434	2438	2442	rBV	94420	141413	4.61%	0.236%
93	15.560	2450	2456	2464	rBV2	223849	384937	12.54%	0.643%
94	15.694	2473	2478	2482	rBV	219382	351723	11.45%	0.587%
95	15.737	2482	2485	2495	rVB	113017	178355	5.81%	0.298%
96	15.926	2508	2516	2526	rBV2	49509	134606	4.38%	0.225%
97	16.078	2537	2541	2546	rBV	30828	47847	1.56%	0.080%
98	16.182	2553	2558	2562	rBV6	23381	43562	1.42%	0.073%
99	16.462	2600	2604	2610	rVB2	20842	44547	1.45%	0.074%
100	16.700	2640	2643	2649	rVB4	22330	41192	1.34%	0.069%

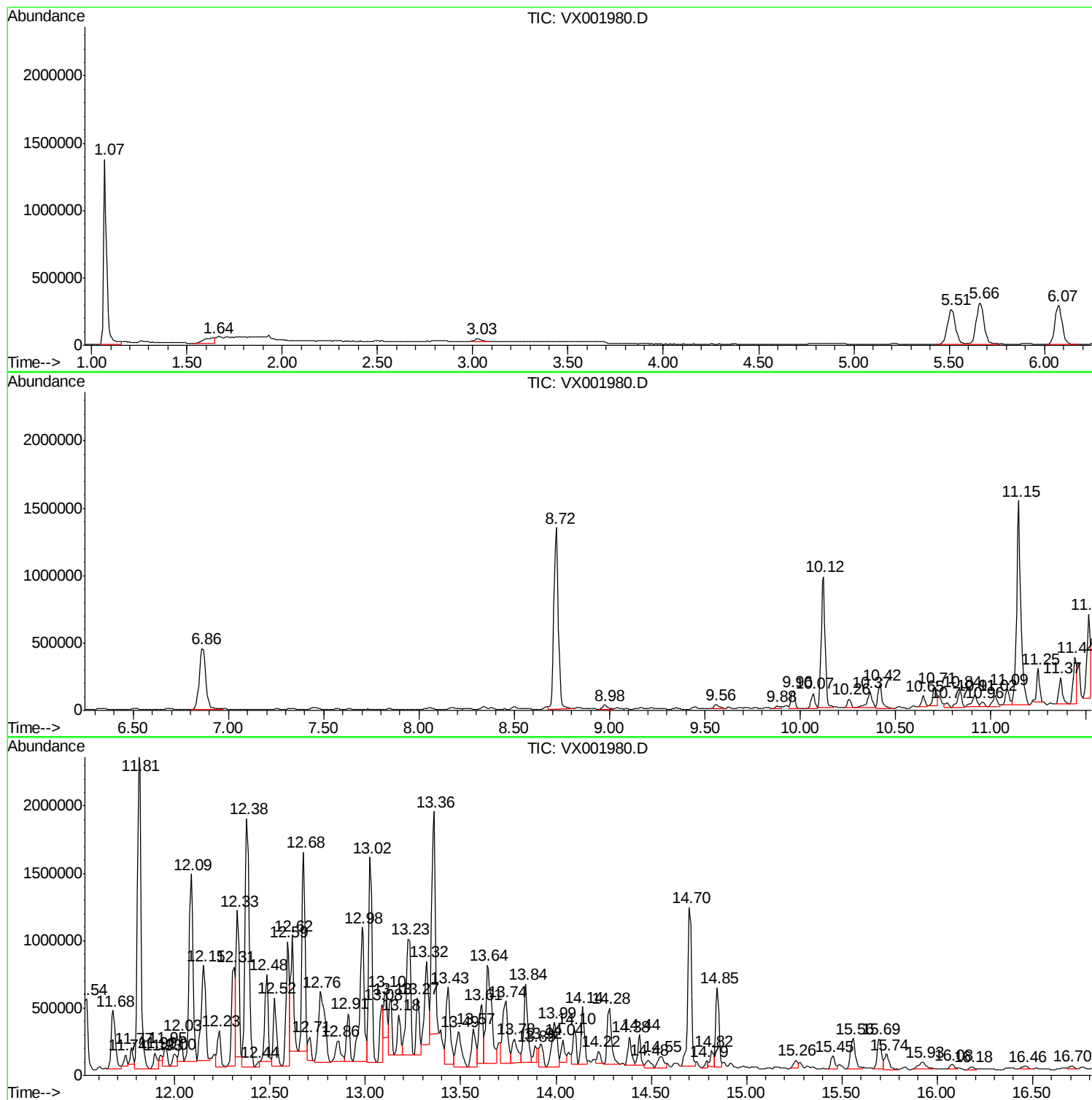
Sum of corrected areas: 59889674

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ALS Vial : 15 Sample Multiplier: 1

Instrument :
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ClientSampleId :
AOC7-BTM-5-5.5

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X052418W.M
Quant Title : SW846 8260

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



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Instrument :
MSVOA_X
ClientSampled :
AOC7-BTM-5-5.5

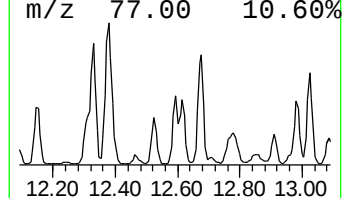
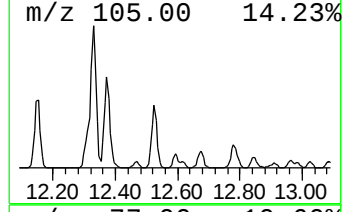
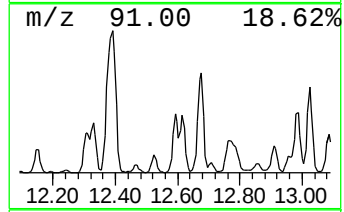
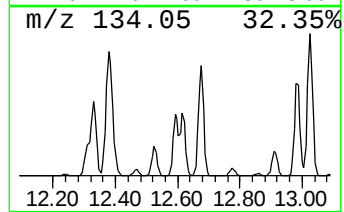
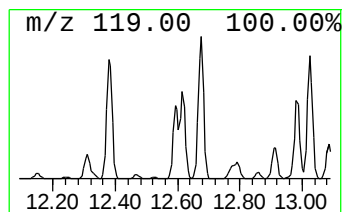
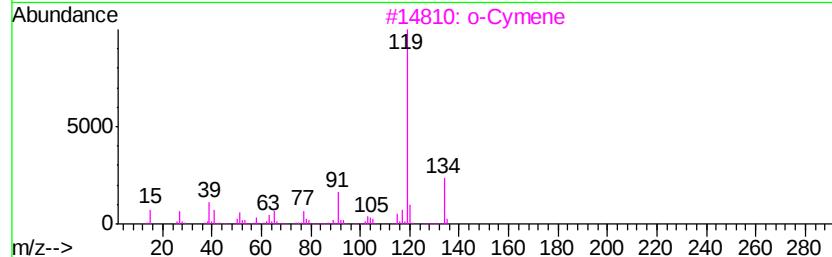
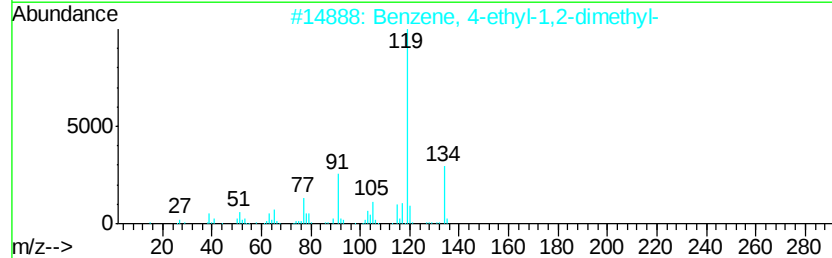
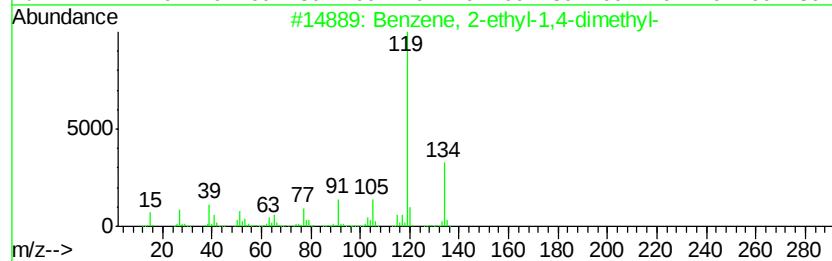
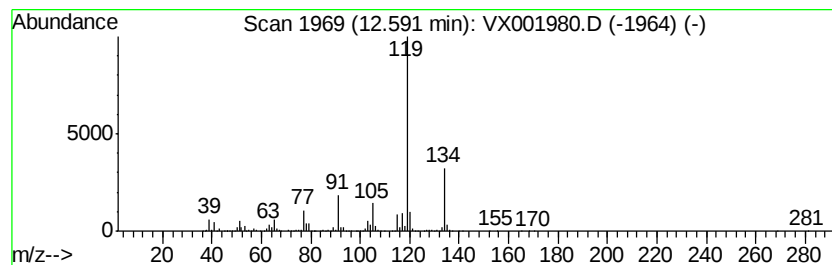
Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X052418W.M
Quant Title : SW846 8260

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

Peak Number 2 Benzene, 2-ethyl-1,4-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.59	30.18 ug/l	1170660	1,4-Dichlorobenzene-d4	12.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	97
2		Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	96
3		o-Cymene	134	C10H14	000527-84-4	95
4		Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95
5		Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	94



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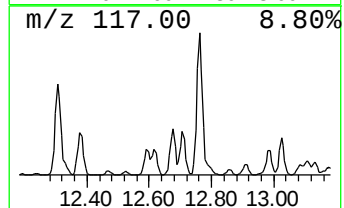
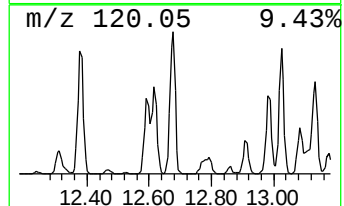
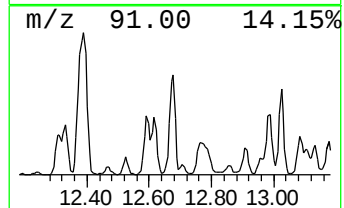
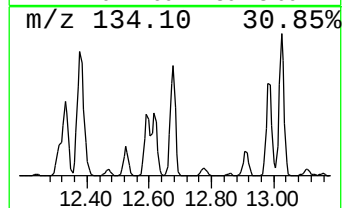
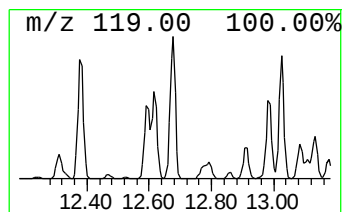
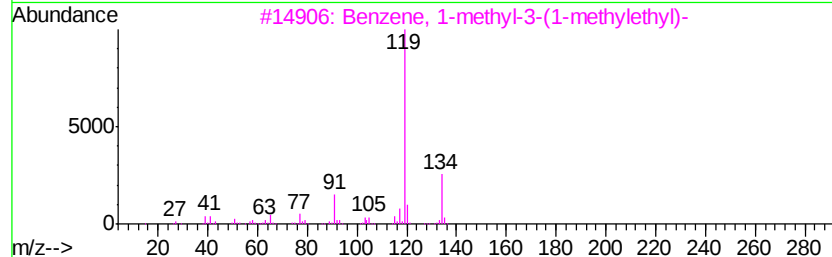
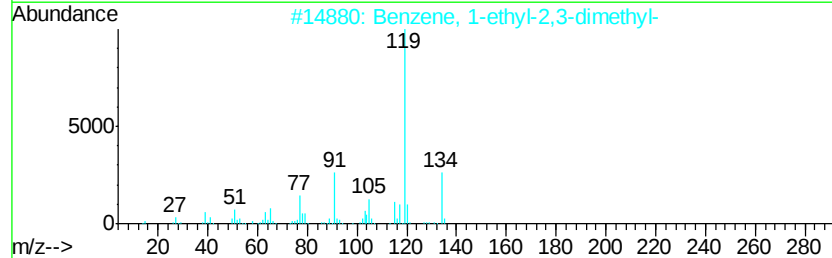
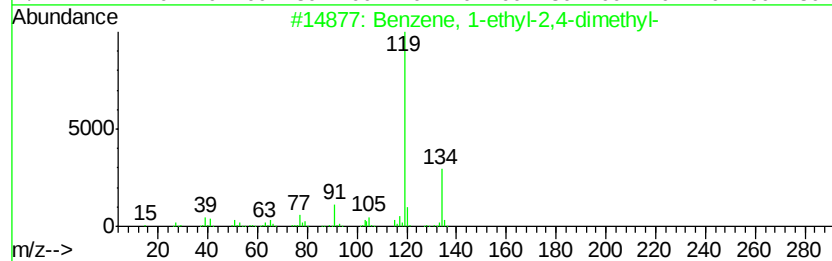
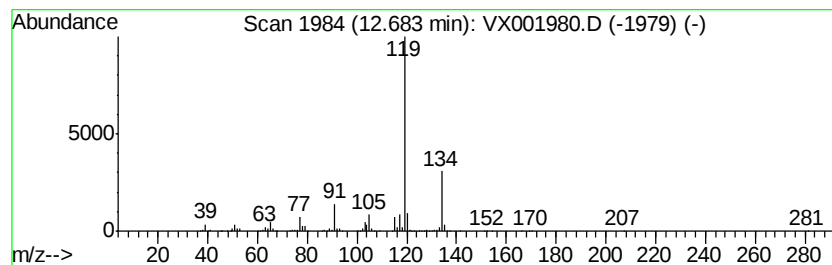
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzene, 1-ethyl-2,4-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.68	43.10 ug/l	1672030	1,4-Dichlorobenzene-d4	12.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	97
2		Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	96
3		Benzene, 1-methyl-3-(1-methylethyl-...)	134	C10H14	000535-77-3	95
4		Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	95
5		Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	95



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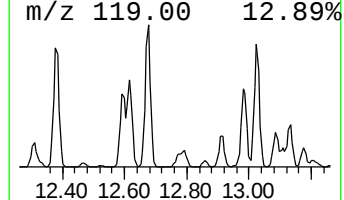
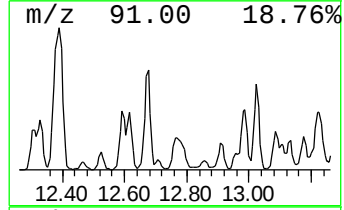
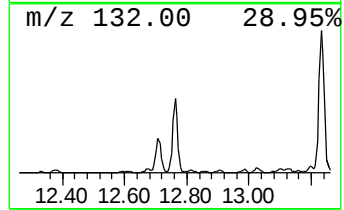
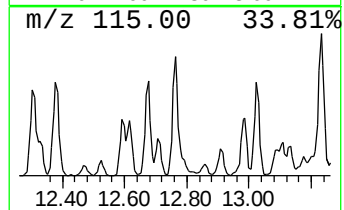
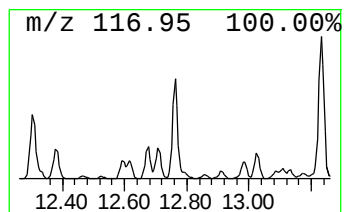
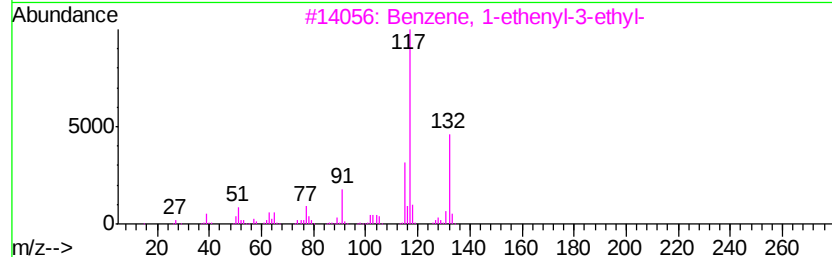
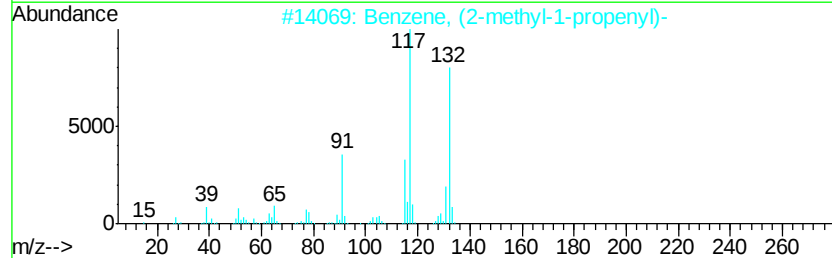
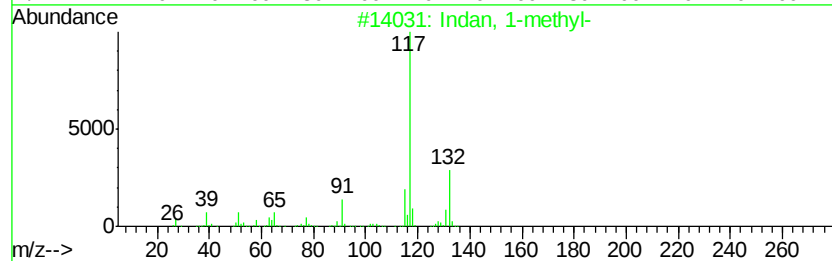
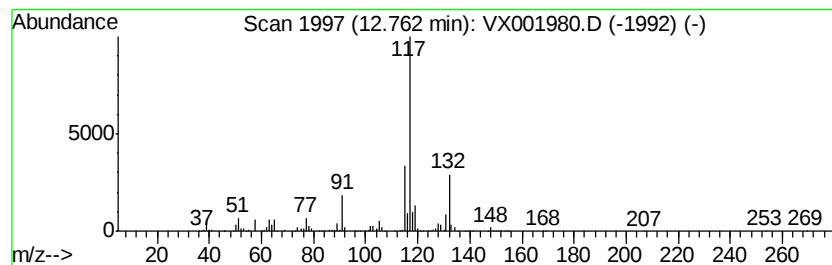
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Quant Title : SW846 8260

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

Peak Number 4 Indan, 1-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.76	32.49 ug/l	1260500	1,4-Dichlorobenzene-d4	12.09

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indan, 1-methyl-		132	C10H12	000767-58-8	94
2	Benzene, (2-methyl-1-propenyl)-		132	C10H12	000768-49-0	91
3	Benzene, 1-ethenyl-3-ethyl-		132	C10H12	007525-62-4	90
4	Benzene, 1-methyl-2-(2-propenyl)-		132	C10H12	001587-04-8	87
5	Benzene, 1-ethenyl-4-ethyl-		132	C10H12	003454-07-7	87



Data Path : W:\HPCHEM1\MSVOA X\DATA\VX052518\
Data File : VX001980.D
Acq On : 25 May 2018 16:36
Operator : JC/MD
Sample : J3015-15
Misc : 5.48g/5mL/100uL/5mL/MSVOA_X/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
AOC7-BTM-5-5.5

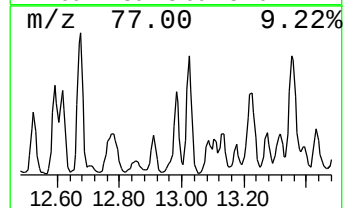
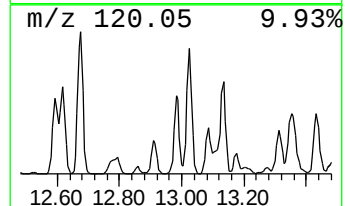
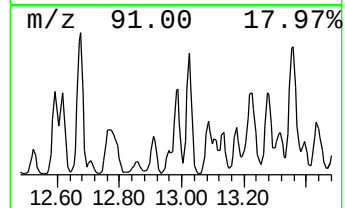
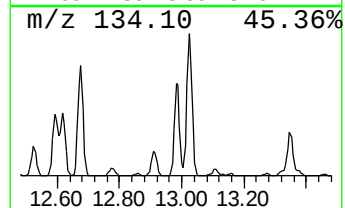
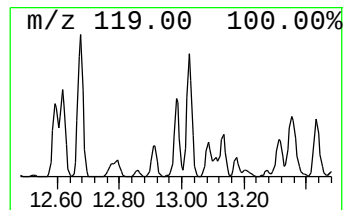
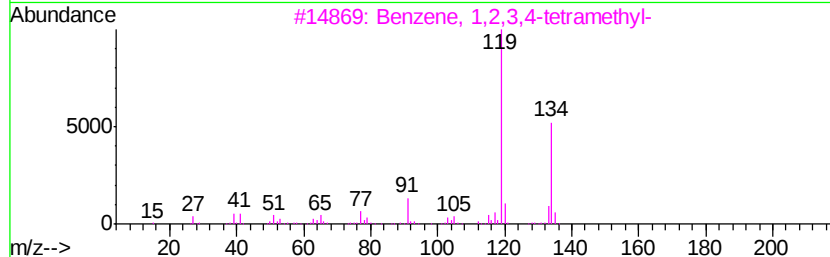
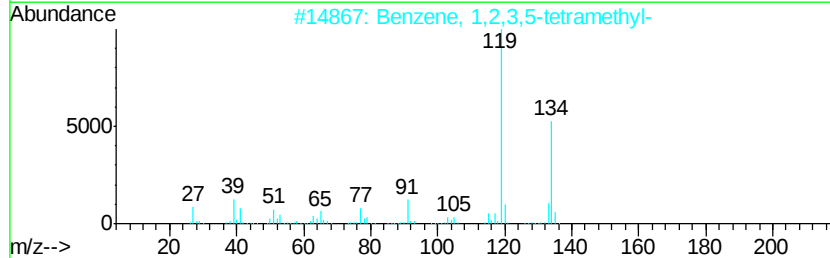
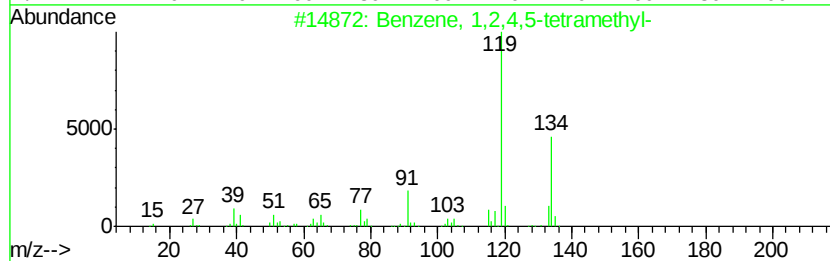
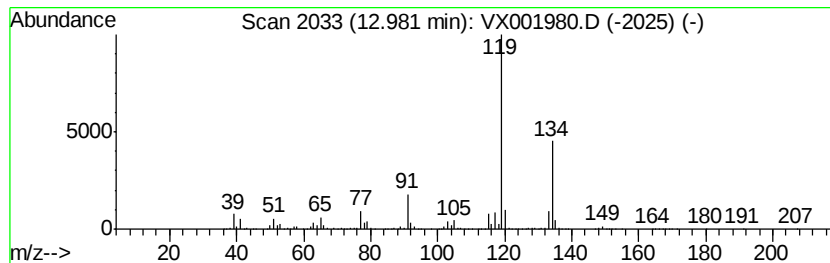
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Quant Title : SW846 8260

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

Peak Number 5 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.98	41.24 ug/l	1600010	1,4-Dichlorobenzene-d4	12.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	96
2		Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	95
3		Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	94
4		Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	93
5		o-Cymene	134	C10H14	000527-84-4	93



Data Path : W:\HPCHEM1\MSVOA X\DATA\VX052518\
Data File : VX001980.D
Acq On : 25 May 2018 16:36
Operator : JC/MD
Sample : J3015-15
Misc : 5.48g/5mL/100uL/5mL/MSVOA_X/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampled :
AOC7-BTM-5-5.5

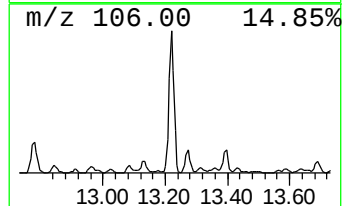
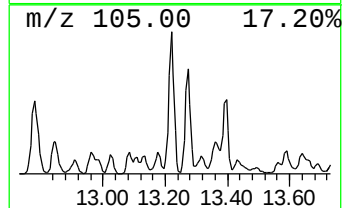
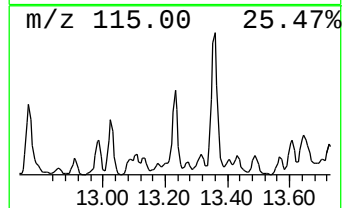
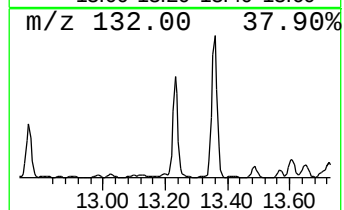
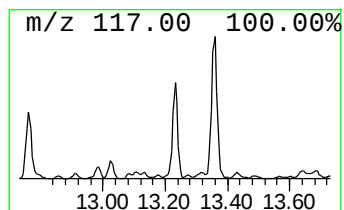
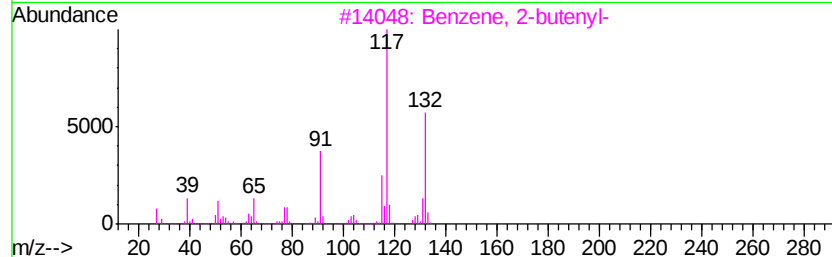
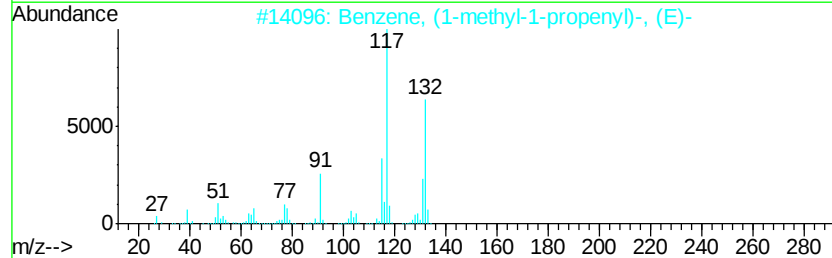
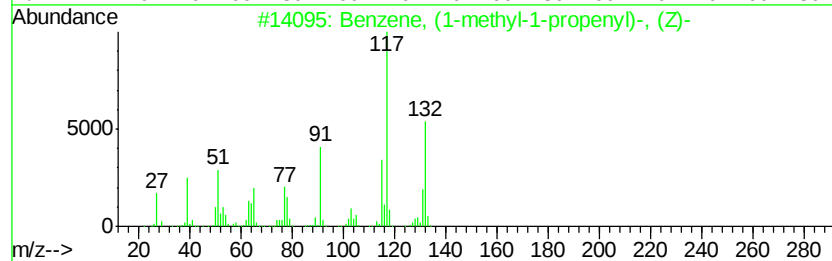
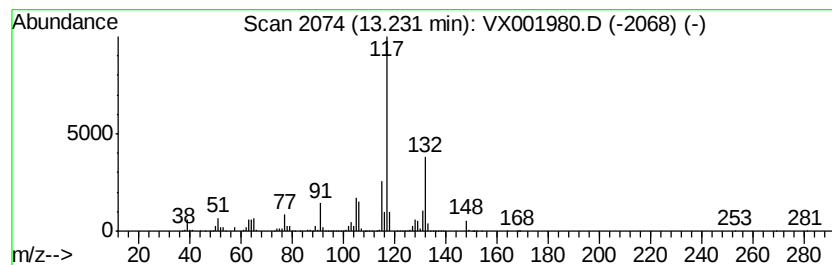
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, (1-methyl-1-propen... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.23	36.62 ug/l	1420630	1,4-Dichlorobenzene-d4	12.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, (1-methyl-1-propenyl)-, ...	132	C10H12	000767-99-7	86
2		Benzene, (1-methyl-1-propenyl)-, ...	132	C10H12	000768-00-3	70
3		Benzene, 2-butenyl-	132	C10H12	001560-06-1	64
4		Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	62
5		Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	62



Data Path : W:\HPCHEM1\MSVOA X\DATA\VX052518\
Data File : VX001980.D
Acq On : 25 May 2018 16:36
Operator : JC/MD
Sample : J3015-15
Misc : 5.48g/5mL/100uL/5mL/MSVOA_X/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
AOC7-BTM-5-5.5

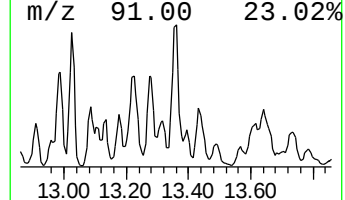
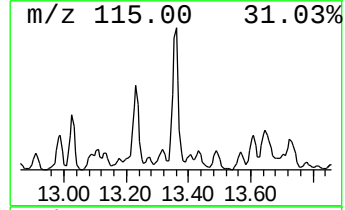
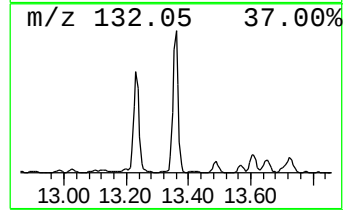
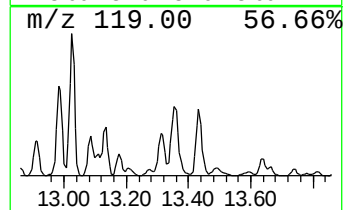
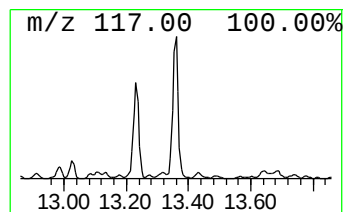
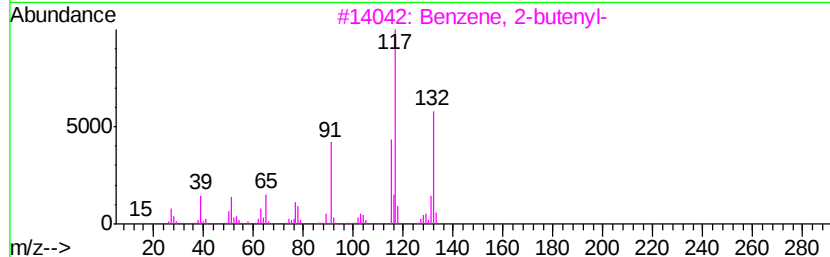
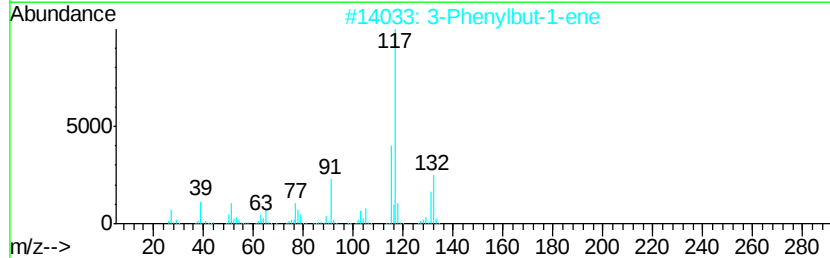
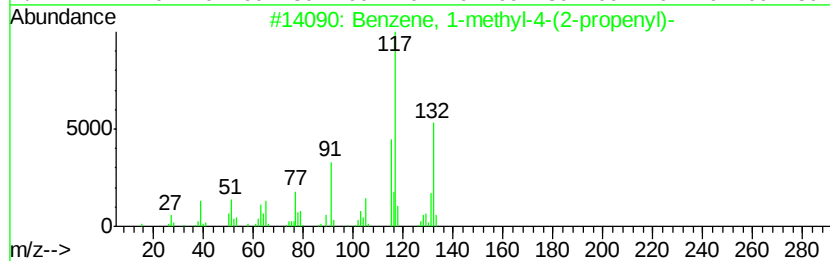
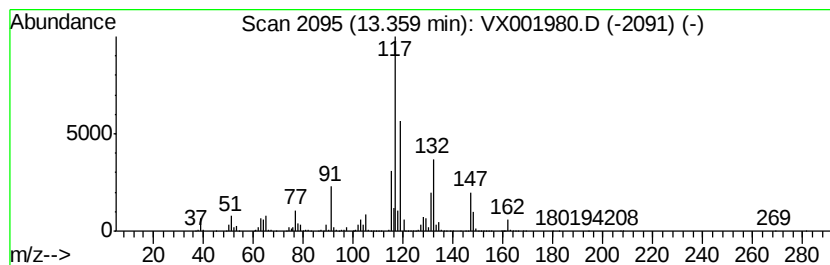
Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X052418W.M
Quant Title : SW846 8260

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

Peak Number 8 Benzene, 1-methyl-4-(2-prop... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.36	56.18 ug/l	2179410	1,4-Dichlorobenzene-d4	12.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	86
2		3-Phenylbut-1-ene	132	C10H12	000934-10-1	83
3		Benzene, 2-butenyl-	132	C10H12	001560-06-1	60
4		1-Phenyl-1-butene	132	C10H12	000824-90-8	60
5		Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	60



Data Path : W:\HPCHEM1\MSVOA X\DATA\VX052518\
Data File : VX001980.D
Acq On : 25 May 2018 16:36
Operator : JC/MD
Sample : J3015-15
Misc : 5.48g/5mL/100uL/5mL/MSVOA_X/MEOH
ALS Vial : 15 Sample Multiplier: 1

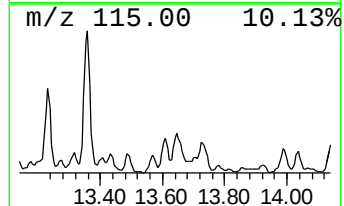
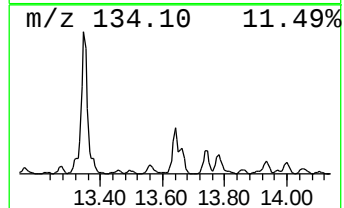
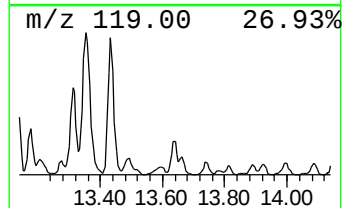
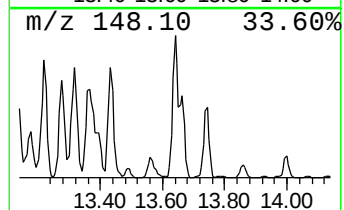
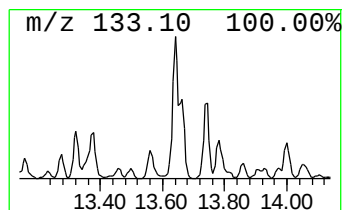
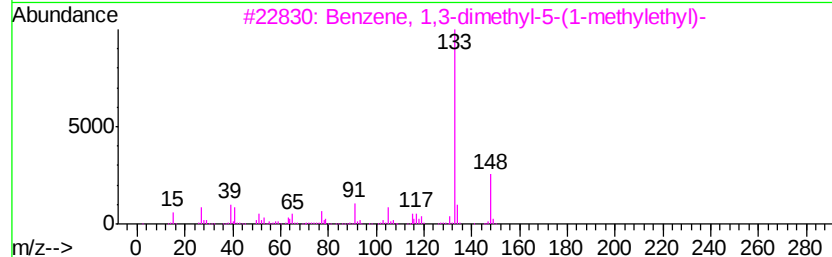
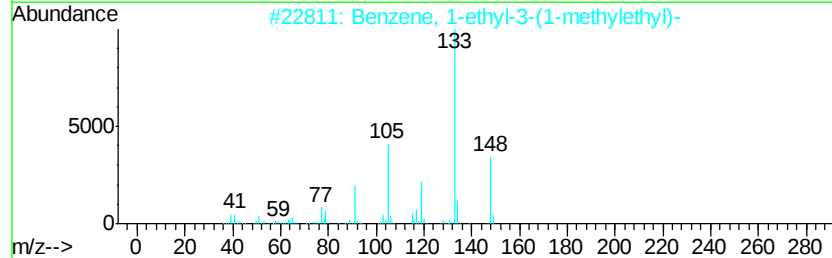
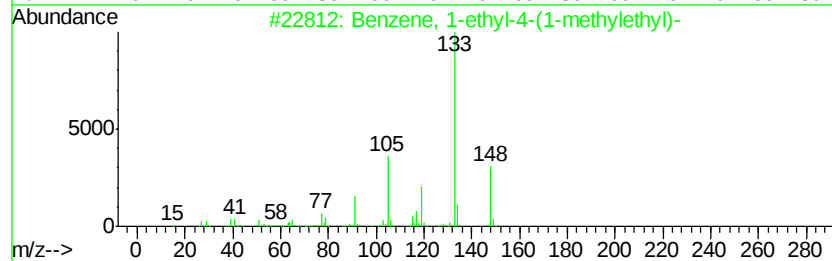
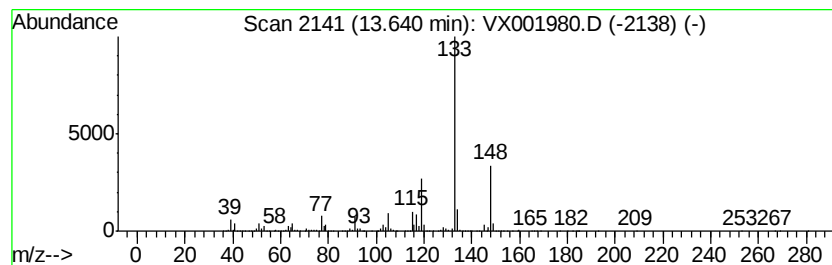
Instrument :
MSVOA_X
ClientSampleId :
AOC7-BTM-5-5.5

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X052418W.M
Quant Title : SW846 8260

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

Peak Number 9 Benzene, 1-ethyl-4-(1-methy... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.64	39.98 ug/l	1551010	1,4-Dichlorobenzene-d4	12.09
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzene, 1-ethyl-4-(1-methylethyl)-	148 C11H16	004218-48-8 91
2		Benzene, 1-ethyl-3-(1-methylethyl)-	148 C11H16	004920-99-4 90
3		Benzene, 1,3-dimethyl-5-(1-methy...	148 C11H16	004706-90-5 87
4		Benzene, 2,4-dimethyl-1-(1-methy...	148 C11H16	004706-89-2 87
5		Benzene, pentamethyl-	148 C11H16	000700-12-9 87



Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX052518\
Data File : VX001980.D
Acq On : 25 May 2018 16:36
Operator : JC/MD
Sample : J3015-15
Misc : 5.48g/5mL/100uL/5mL/MSVOA_X/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
AOC7-BTM-5-5.5

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X052418W.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
Benzene, 2-ethyl-...	12.59	30.2	ug/l	1170660	4	12.09	1939650	50.0
Benzene, 1-ethyl-...	12.68	43.1	ug/l	1672030	4	12.09	1939650	50.0
Indan, 1-methyl-	12.76	32.5	ug/l	1260500	4	12.09	1939650	50.0
Benzene, 1,2,4,5-...	12.98	41.2	ug/l	1600010	4	12.09	1939650	50.0
Benzene, (1-methy...	13.23	36.6	ug/l	1420630	4	12.09	1939650	50.0
Benzene, 1-methyl...	13.36	56.2	ug/l	2179410	4	12.09	1939650	50.0
Benzene, 1-ethyl-...	13.64	40.0	ug/l	1551010	4	12.09	1939650	50.0