

Data Path : W:\HPCHEM1\MSVOA X\DATA\VX052518\
 Data File : VX001986.D
 Acq On : 25 May 2018 19:16
 Operator : JC/MD
 Sample : J3064-02
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-16

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	1.075	76	80	93	rBV	2978684	3585541	100.00%	10.340%
2	1.343	118	124	140	rBV2	72335	439993	12.27%	1.269%
3	2.453	301	306	313	rVB	24133	40963	1.14%	0.118%
4	2.630	329	335	343	rBV	38938	70615	1.97%	0.204%
5	3.215	426	431	439	rVB2	18311	43295	1.21%	0.125%
6	5.513	795	808	822	rBV	272118	782049	21.81%	2.255%
7	5.672	822	834	846	rVV	317287	878314	24.50%	2.533%
8	6.074	890	900	920	rBV	303420	794913	22.17%	2.292%
9	6.867	1019	1030	1049	rBV	476389	1134513	31.64%	3.272%
10	8.720	1327	1334	1343	rBV	1374908	2158691	60.21%	6.225%
11	10.116	1554	1563	1570	rBV	984972	1381041	38.52%	3.982%
12	10.189	1572	1575	1581	rVB	23054	35911	1.00%	0.104%
13	10.342	1595	1600	1609	rVB4	23441	55499	1.55%	0.160%
14	10.665	1647	1653	1657	rVB5	21311	44380	1.24%	0.128%
15	10.841	1679	1682	1691	rVB2	31188	38732	1.08%	0.112%
16	10.939	1691	1698	1707	rBV9	27721	93627	2.61%	0.270%
17	11.024	1707	1712	1725	rVB	210450	303485	8.46%	0.875%
18	11.140	1726	1731	1737	rBV	1215369	1615040	45.04%	4.657%
19	11.286	1751	1755	1762	rVB3	24701	39076	1.09%	0.113%
20	11.366	1763	1768	1777	rVB	247538	317274	8.85%	0.915%
21	11.701	1815	1823	1827	rBV7	31525	70218	1.96%	0.202%
22	11.774	1831	1835	1838	rBV	60839	76649	2.14%	0.221%
23	11.927	1852	1860	1861	rBV	90211	123675	3.45%	0.357%
24	11.951	1861	1864	1874	rVB	248706	331894	9.26%	0.957%
25	12.085	1880	1886	1891	rBV	1202686	1529602	42.66%	4.411%
26	12.189	1898	1903	1906	rBV5	30981	55895	1.56%	0.161%
27	12.238	1907	1911	1915	rVV	145610	183751	5.12%	0.530%
28	12.305	1915	1922	1926	rVV	714802	895603	24.98%	2.583%
29	12.372	1930	1933	1943	rVB2	185042	355061	9.90%	1.024%
30	12.463	1943	1948	1953	rBV	384566	498374	13.90%	1.437%
31	12.670	1975	1982	1986	rBV	453644	584987	16.32%	1.687%
32	12.707	1986	1988	1993	rVV2	107855	162971	4.55%	0.470%
33	12.762	1993	1997	2004	rVV3	557572	1025296	28.60%	2.957%
34	12.817	2004	2006	2010	rVB2	113159	131117	3.66%	0.378%

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35	12.902	2010	2020	2024	rVB3	220781	410145	11.44%	1.183%
36	12.981	2024	2033	2038	rBV	793846	1140043	31.80%	3.288%
37	13.036	2039	2042	2046	rVB2	31413	48453	1.35%	0.140%
38	13.091	2046	2051	2056	rVB3	156244	247001	6.89%	0.712%
39	13.158	2056	2062	2065	rBV	127285	193491	5.40%	0.558%
40	13.201	2065	2069	2072	rVV	319853	390450	10.89%	1.126%
41	13.231	2072	2074	2076	rVV	90367	91793	2.56%	0.265%
42	13.256	2076	2078	2083	rVB	105038	126689	3.53%	0.365%
43	13.317	2083	2088	2090	rBV2	127548	190540	5.31%	0.549%
44	13.353	2090	2094	2100	rVB2	822443	1194130	33.30%	3.444%
45	13.408	2100	2103	2105	rBV3	54156	63640	1.77%	0.184%
46	13.432	2105	2107	2109	rVB	46564	36722	1.02%	0.106%
47	13.487	2109	2116	2121	rBV5	112787	202295	5.64%	0.583%
48	13.536	2121	2124	2127	rVV3	40801	46870	1.31%	0.135%
49	13.567	2127	2129	2132	rVV3	65741	85571	2.39%	0.247%
50	13.609	2132	2136	2138	rVV	175831	231425	6.45%	0.667%
51	13.646	2138	2142	2146	rVV3	344079	512535	14.29%	1.478%
52	13.707	2146	2152	2153	rVV2	282925	456526	12.73%	1.316%
53	13.731	2153	2156	2162	rVV3	373445	727438	20.29%	2.098%
54	13.817	2166	2170	2173	rBV	109784	159894	4.46%	0.461%
55	13.859	2173	2177	2182	rVB3	149482	222478	6.20%	0.642%
56	13.914	2182	2186	2191	rBV	313296	440527	12.29%	1.270%
57	13.987	2192	2198	2202	rVV2	389689	564897	15.75%	1.629%
58	14.036	2202	2206	2214	rVB3	189690	381441	10.64%	1.100%
59	14.140	2218	2223	2225	rBV2	131297	199775	5.57%	0.576%
60	14.164	2225	2227	2231	rVB2	120278	141459	3.95%	0.408%
61	14.225	2231	2237	2241	rBV8	67630	139799	3.90%	0.403%
62	14.274	2241	2245	2257	rBV4	306001	584429	16.30%	1.685%
63	14.383	2258	2263	2267	rVB2	269118	426057	11.88%	1.229%
64	14.438	2267	2272	2276	rBV4	211591	322098	8.98%	0.929%
65	14.481	2276	2279	2282	rBV	44016	62833	1.75%	0.181%
66	14.548	2286	2290	2293	rBV2	419622	563529	15.72%	1.625%
67	14.579	2293	2295	2299	rVB2	106128	126768	3.54%	0.366%
68	14.640	2302	2305	2308	rBV2	49013	64847	1.81%	0.187%
69	14.676	2308	2311	2314	rBV4	89383	130208	3.63%	0.375%
70	14.737	2318	2321	2324	rVB	67206	71785	2.00%	0.207%
71	14.853	2336	2340	2343	rBV	128275	198377	5.53%	0.572%

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72	14.969	2353	2359	2366	rBV8	144514	422868	11.79%	1.219%
73	15.036	2366	2370	2372	rBV5	89915	135112	3.77%	0.390%
74	15.127	2381	2385	2389	rVB2	125488	163691	4.57%	0.472%
75	15.255	2399	2406	2410	rBV3	187526	486068	13.56%	1.402%
76	15.402	2425	2430	2435	rBV	406032	608266	16.96%	1.754%
77	15.487	2440	2444	2451	rVB4	93260	211409	5.90%	0.610%
78	15.560	2451	2456	2460	rBV	184930	279358	7.79%	0.806%
79	15.694	2471	2478	2483	rBV2	240752	470255	13.12%	1.356%
80	15.816	2492	2498	2504	rBV3	90549	205623	5.73%	0.593%
81	15.895	2508	2511	2514	rBV3	54843	87785	2.45%	0.253%
82	16.078	2537	2541	2553	rVB2	132502	276723	7.72%	0.798%
83	16.182	2554	2558	2568	rVB4	55327	118833	3.31%	0.343%
84	16.572	2617	2622	2628	rVB2	75927	136759	3.81%	0.394%

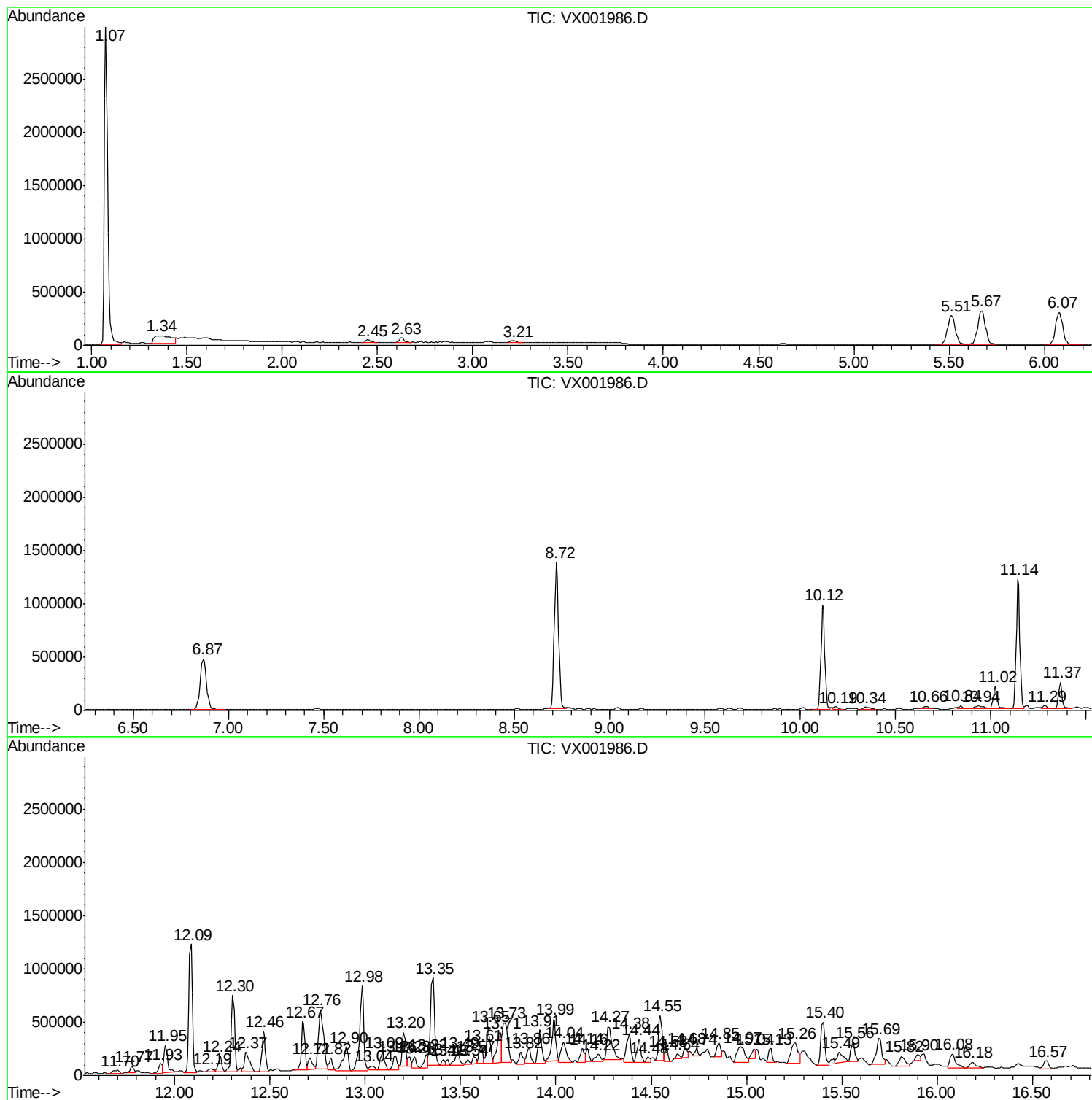
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Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X052418W.M
Quant Title : SW846 8260

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



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Instrument :
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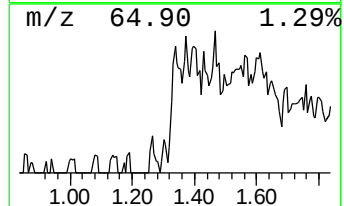
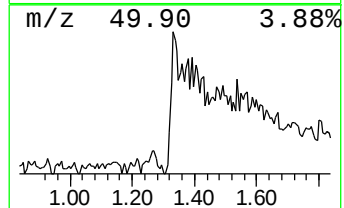
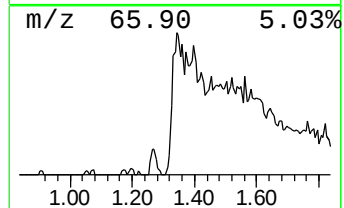
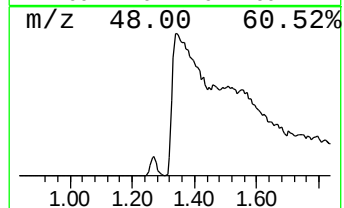
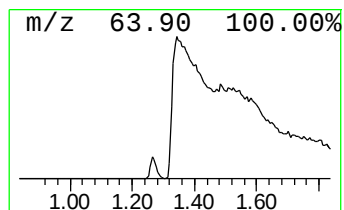
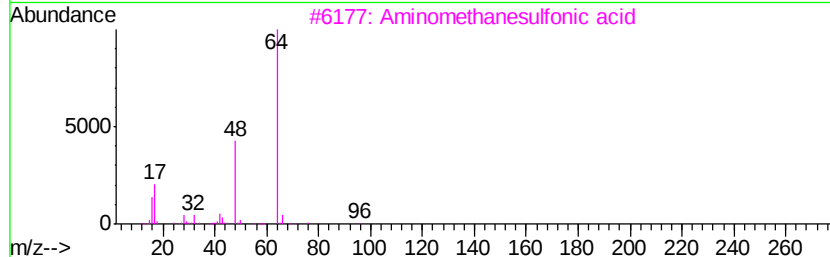
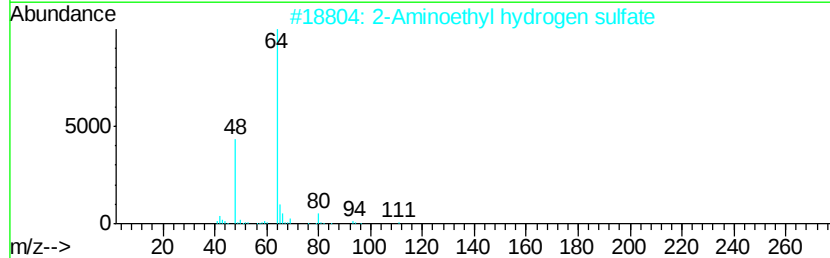
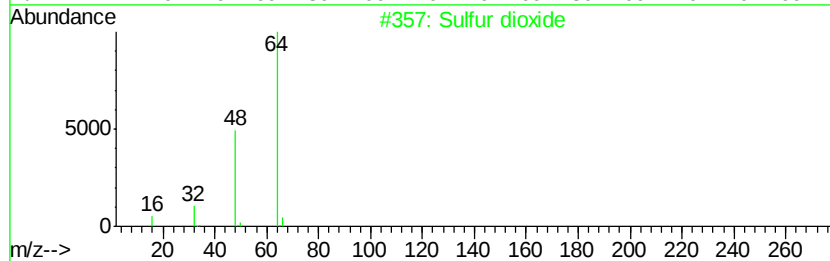
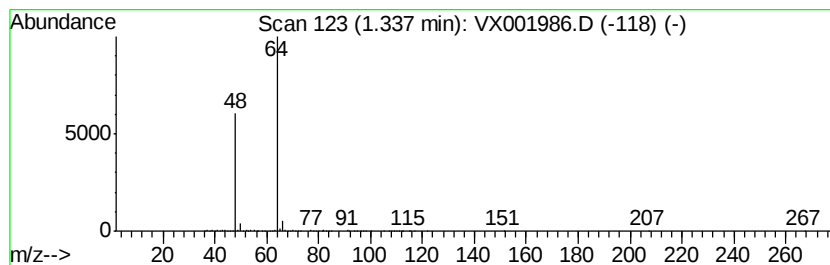
Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X052418W.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Sulfur dioxide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.34	25.05 ug/l	439993	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Sulfur dioxide	64	O2S	007446-09-5	83
2		2-Aminoethyl hydrogen sulfate	141	C2H7N04S	000926-39-6	74
3		Aminomethanesulfonic acid	111	CH5N03S	013881-91-9	74
4		L-Alanine, 3-sulfo-	169	C3H7N05S	000498-40-8	64
5		(N-(-2-Acetamido))-2-aminoethane...	182	C4H10N2O4S	007365-82-4	9



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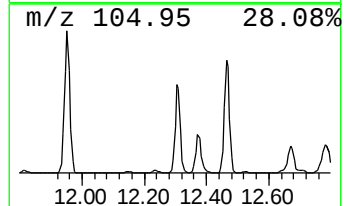
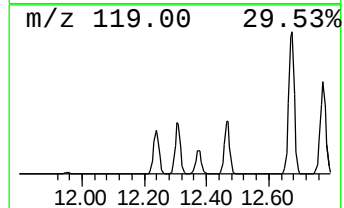
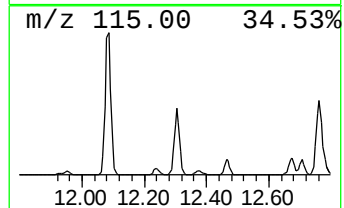
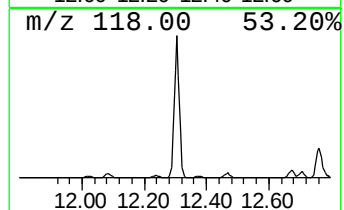
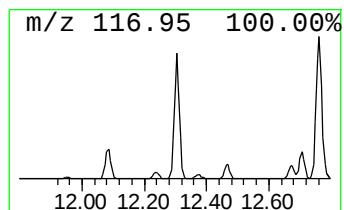
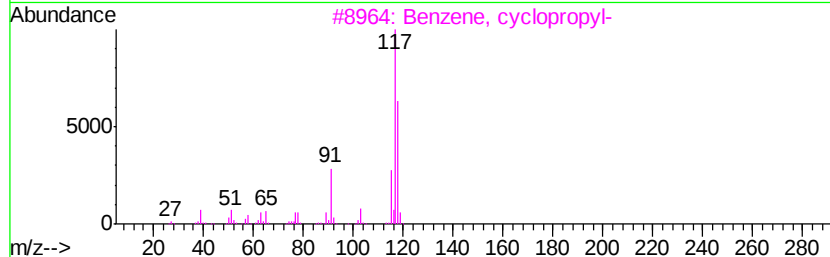
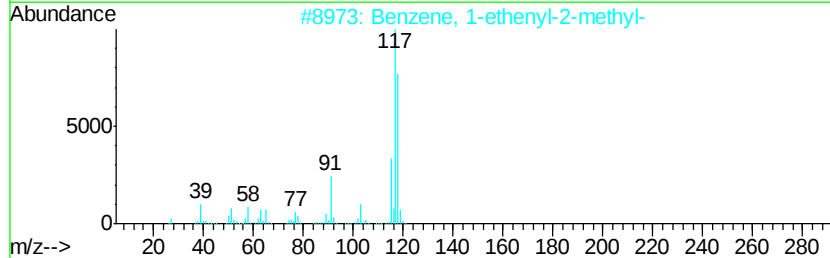
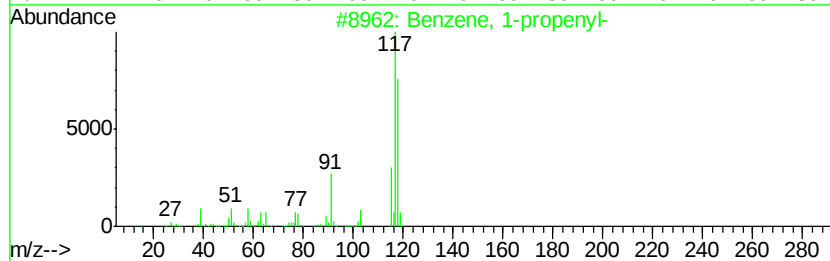
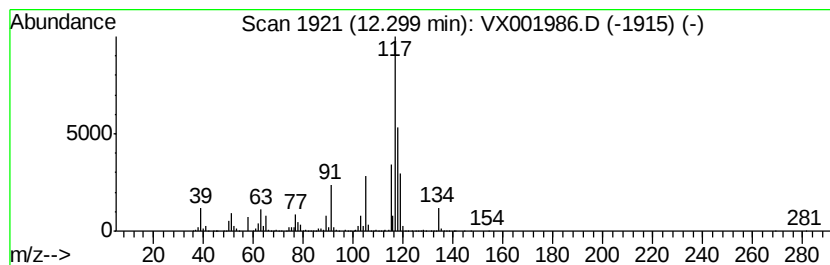
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzene, 1-propenyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.30	29.28 ug/l	895603	1,4-Dichlorobenzene-d4	12.09

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzene, 1-propenyl-	118	C9H10	000637-50-3	90
2		Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	60
3		Benzene, cyclopropyl-	118	C9H10	000873-49-4	60
4		Benzene, 2-propenyl-	118	C9H10	000300-57-2	60
5		Indane	118	C9H10	000496-11-7	60



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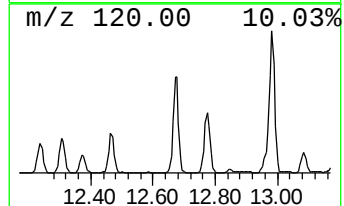
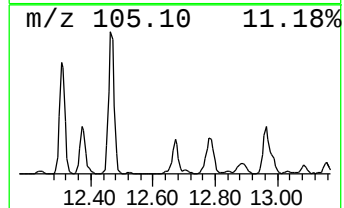
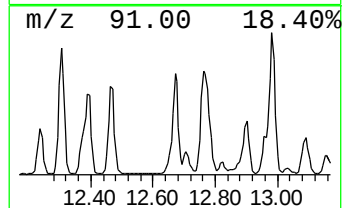
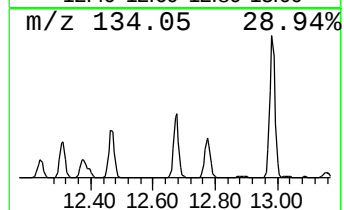
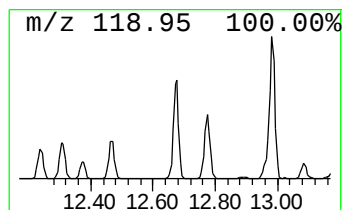
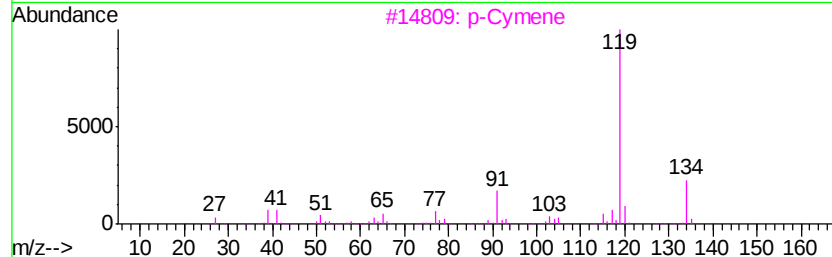
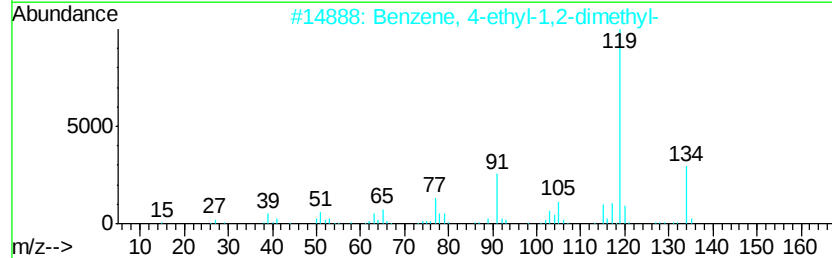
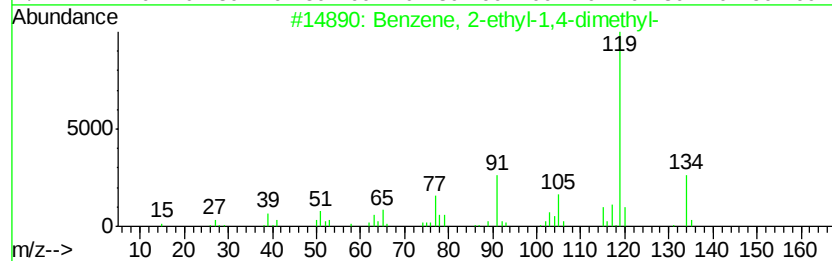
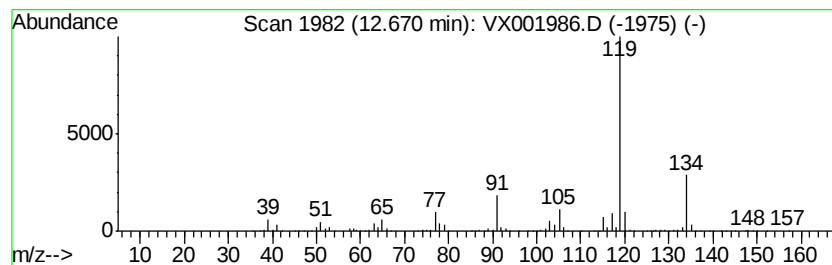
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzene, 2-ethyl-1,4-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.67	19.12 ug/l	584987	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	96
2		Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	96
3		p-Cymene	134	C10H14	000099-87-6	95
4		Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	95
5		o-Cymene	134	C10H14	000527-84-4	95



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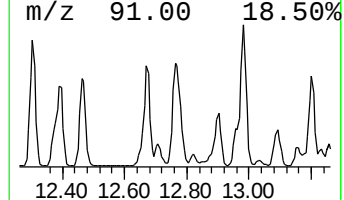
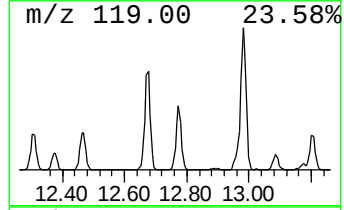
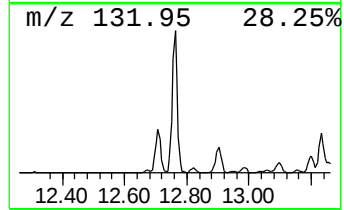
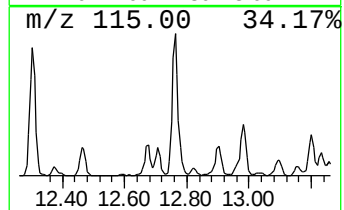
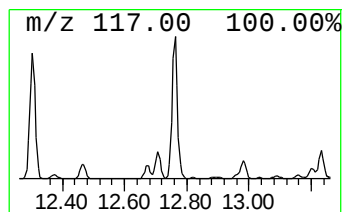
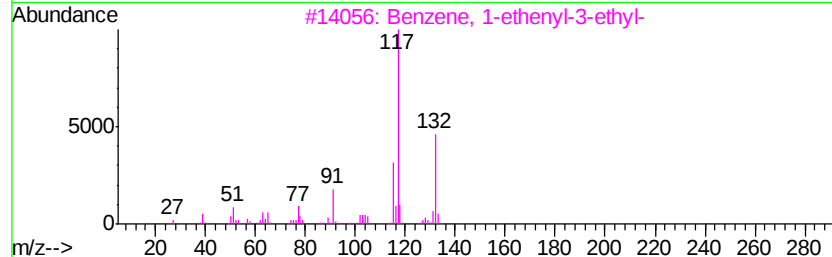
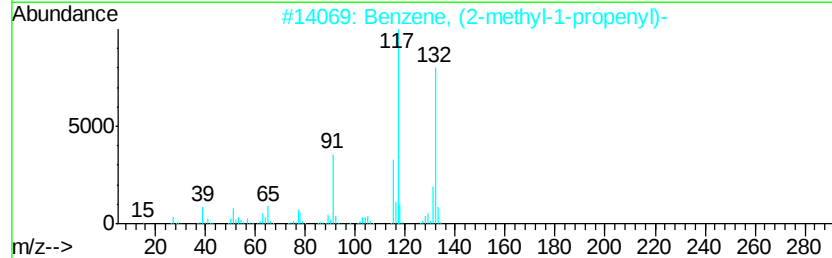
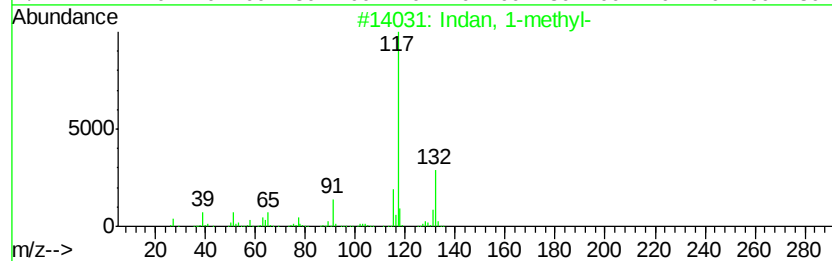
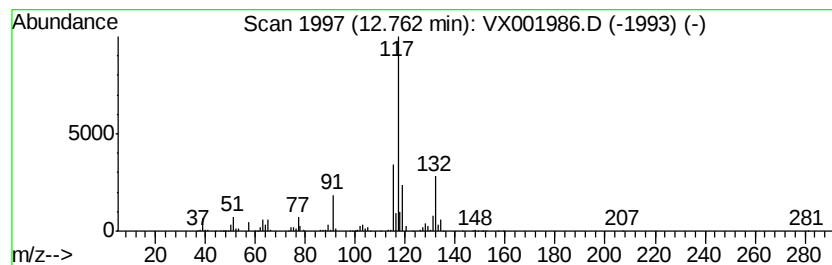
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Quant Title : SW846 8260

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

Peak Number 5 Indan, 1-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.76	33.52 ug/l	1025300	1,4-Dichlorobenzene-d4	12.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Indan, 1-methyl-	132	C10H12	000767-58-8	93
2		Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	87
3		Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	81
4		Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	81
5		Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	76



Data Path : W:\HPCHEM1\MSVOA X\DATA\VX052518\
Data File : VX001986.D
Acq On : 25 May 2018 19:16
Operator : JC/MD
Sample : J3064-02
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-16

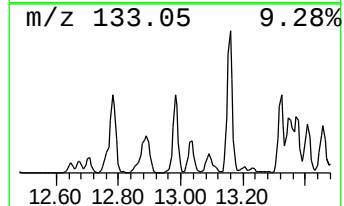
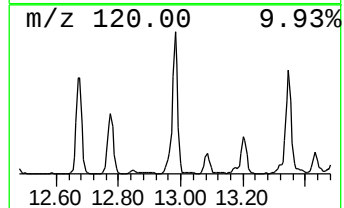
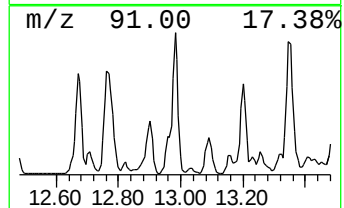
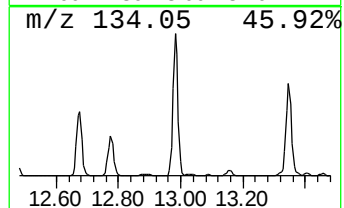
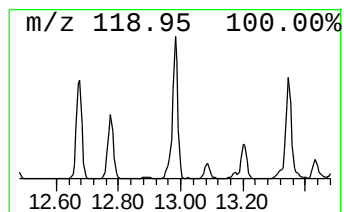
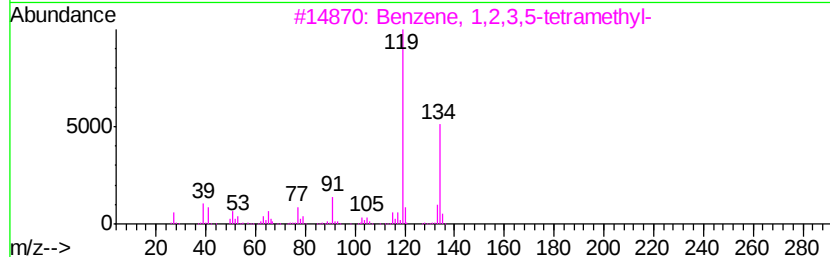
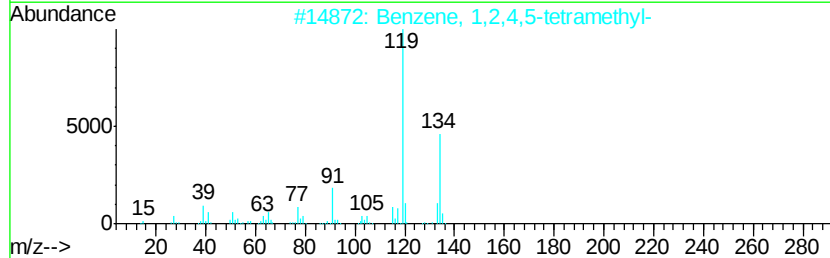
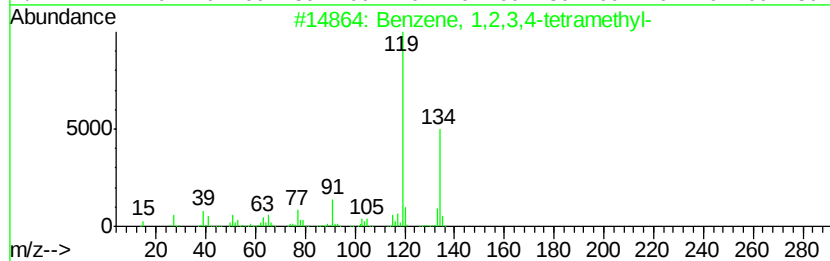
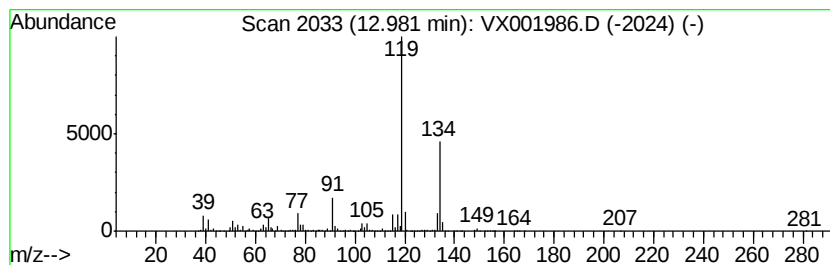
Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X052418W.M
Quant Title : SW846 8260

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

Peak Number 6 Benzene, 1,2,3,4-tetramethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.98	37.27 ug/l	1140040	1,4-Dichlorobenzene-d4	12.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	97
2		Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	96
3		Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	95
4		Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	94
5		o-Cymene	134	C10H14	000527-84-4	93



Data Path : W:\HPCHEM1\MSVOA X\DATA\VX052518\
Data File : VX001986.D
Acq On : 25 May 2018 19:16
Operator : JC/MD
Sample : J3064-02
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-16

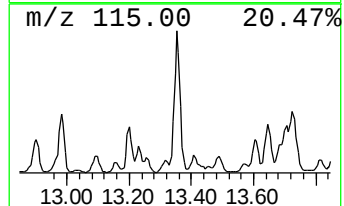
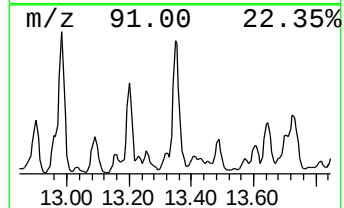
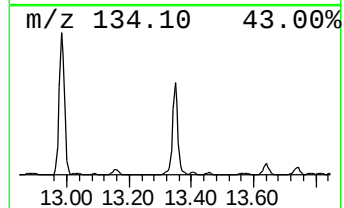
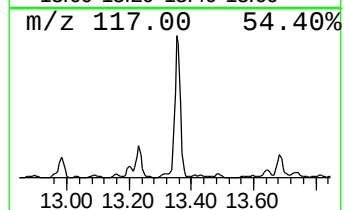
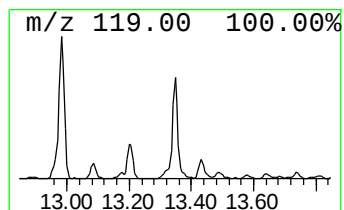
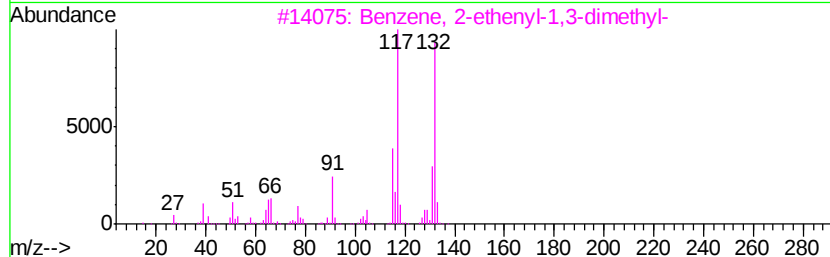
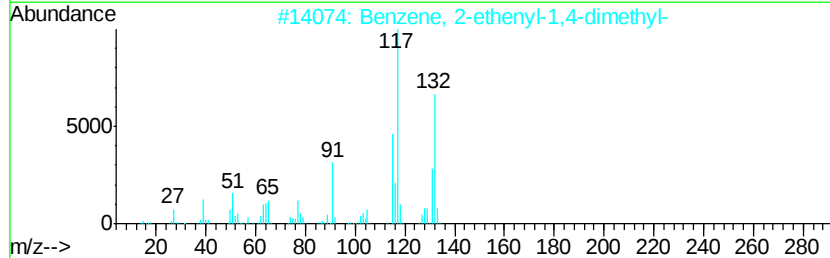
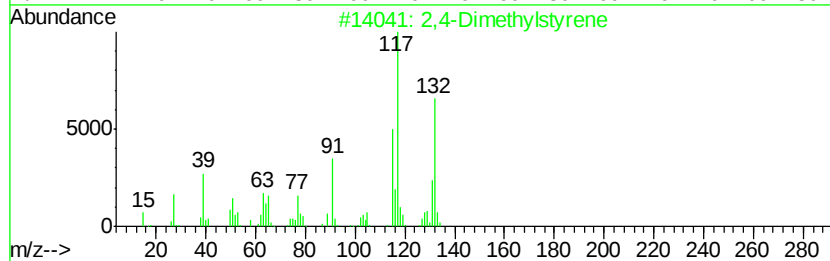
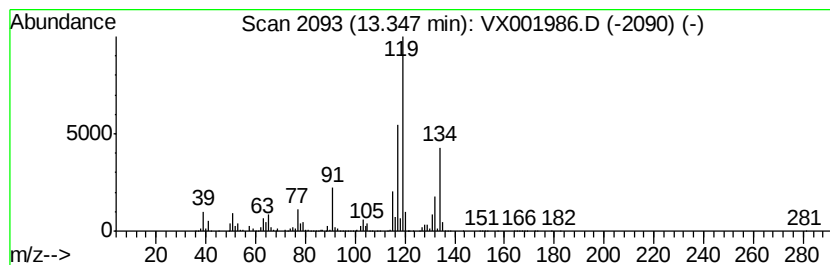
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Quant Title : SW846 8260

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

Peak Number 7 2,4-Dimethylstyrene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.35	39.03 ug/l	1194130	1,4-Dichlorobenzene-d4	12.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2,4-Dimethylstvrene	132	C10H12	002234-20-0	66
2		Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	62
3		Benzene, 2-ethenyl-1,3-dimethyl-	132	C10H12	002039-90-9	60
4		Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000767-99-7	60
5		1-Phenyl-1-butene	132	C10H12	000824-90-8	60



Data Path : W:\HPCHEM1\MSVOA X\DATA\VX052518\
Data File : VX001986.D
Acq On : 25 May 2018 19:16
Operator : JC/MD
Sample : J3064-02
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-16

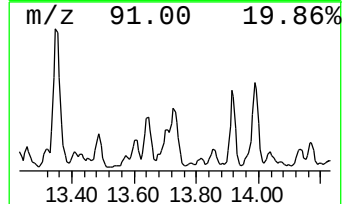
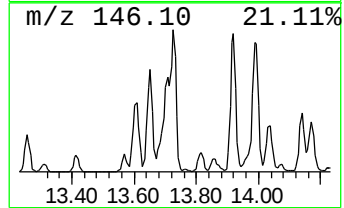
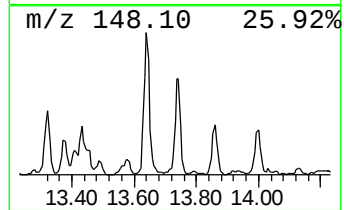
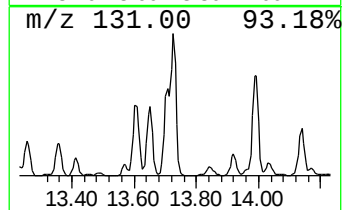
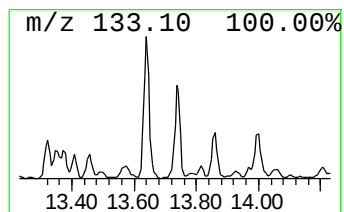
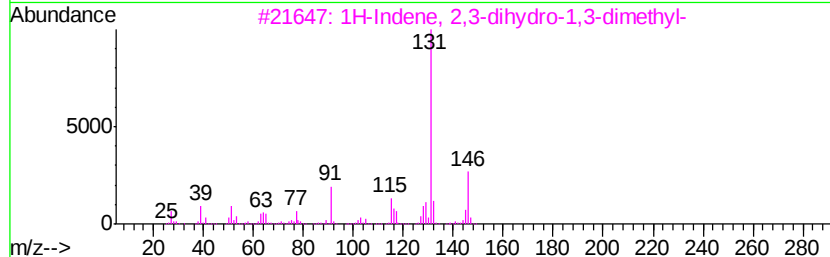
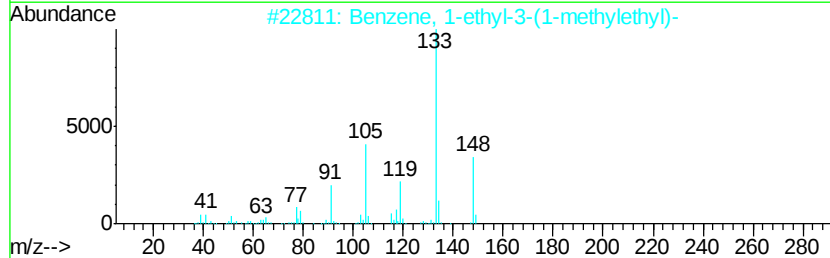
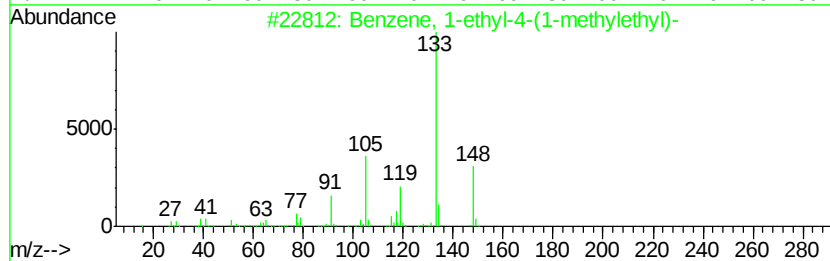
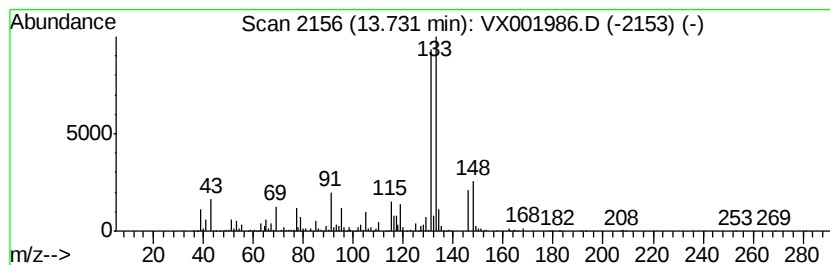
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Quant Title : SW846 8260

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

Peak Number 8 unknown13.73 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	23.78 ug/l	727438	1,4-Dichlorobenzene-d4	12.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-ethyl-4-(1-methylethyl)-	148	C11H16	004218-48-8	45
2		Benzene, 1-ethyl-3-(1-methylethyl)-	148	C11H16	004920-99-4	43
3		1H-Indene, 2,3-dihydro-1,3-dimet...	146	C11H14	004175-53-5	41
4		Benzene, 2,4-dimethyl-1-(1-methy...	148	C11H16	004706-89-2	41
5		Benzene, 1,3-dimethyl-5-(1-methy...	148	C11H16	004706-90-5	41



Data Path : W:\HPCHEM1\MSVOA X\DATA\VX052518\
Data File : VX001986.D
Acq On : 25 May 2018 19:16
Operator : JC/MD
Sample : J3064-02
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-16

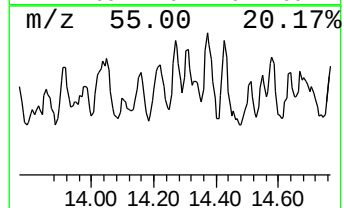
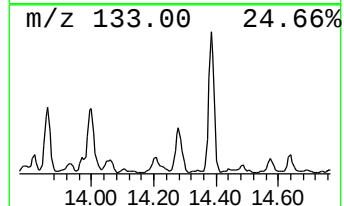
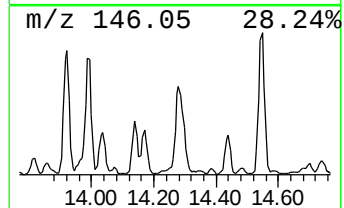
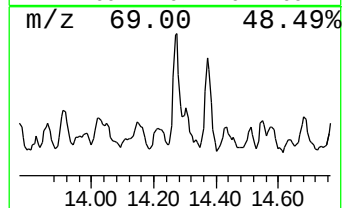
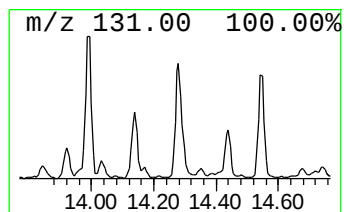
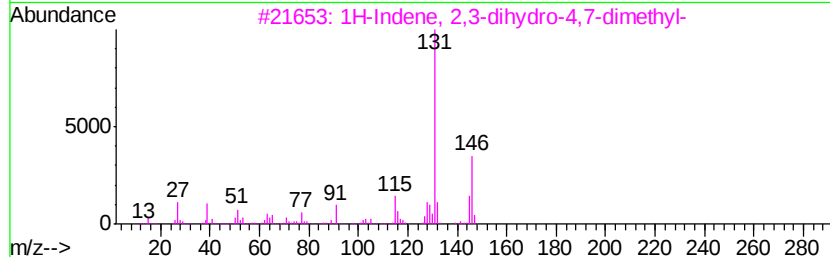
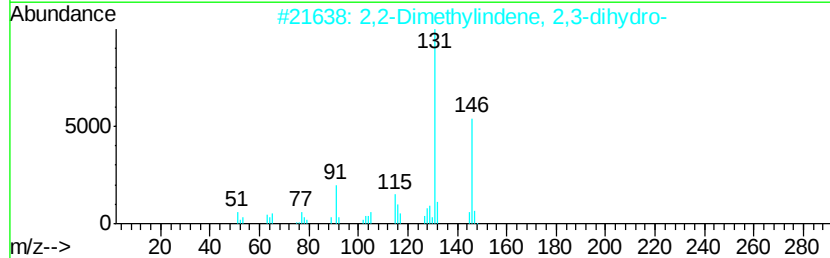
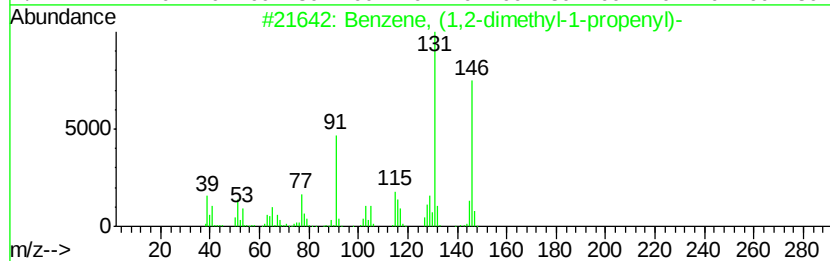
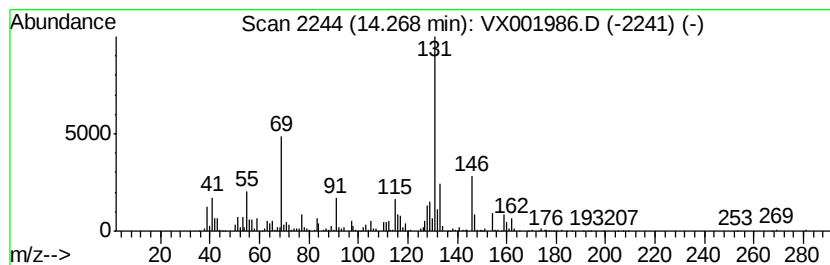
Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X052418W.M
Quant Title : SW846 8260

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

Peak Number 9 Benzene, (1,2-dimethyl-1-propenyl)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.27	19.10 ug/l	584429	1,4-Dichlorobenzene-d4	12.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, (1,2-dimethyl-1-propenyl)-	146	C11H14	000769-57-3	95
2		2,2-Dimethylindene, 2,3-dihydro-	146	C11H14	020836-11-7	91
3		1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	87
4		1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	87
5		Naphthalene, 1,2,3,4-tetrahydro-	146	C11H14	001559-81-5	80



Data Path : W:\HPCHEM1\MSVOA X\DATA\VX052518\
Data File : VX001986.D
Acq On : 25 May 2018 19:16
Operator : JC/MD
Sample : J3064-02
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampled :
MW-16

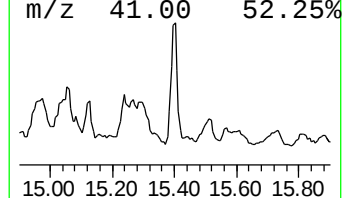
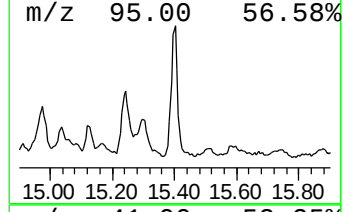
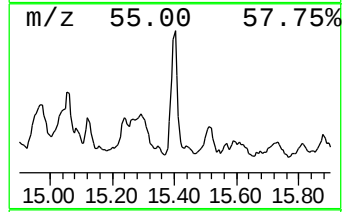
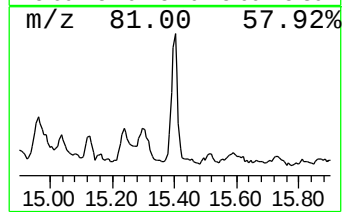
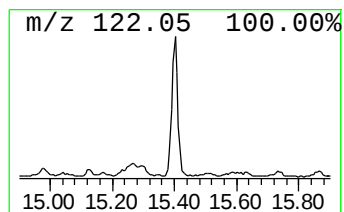
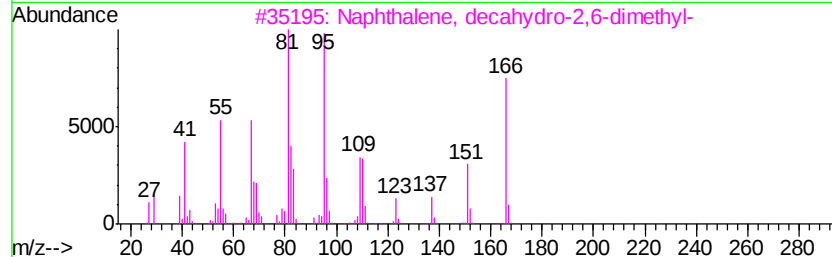
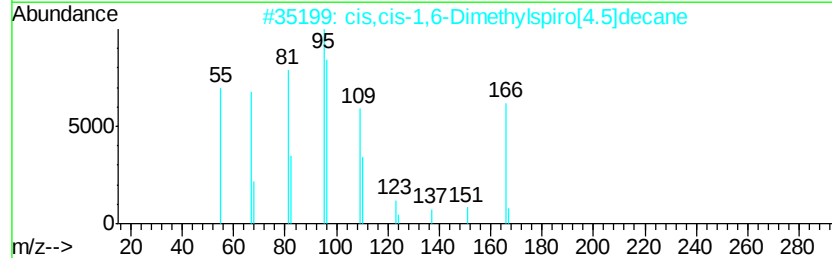
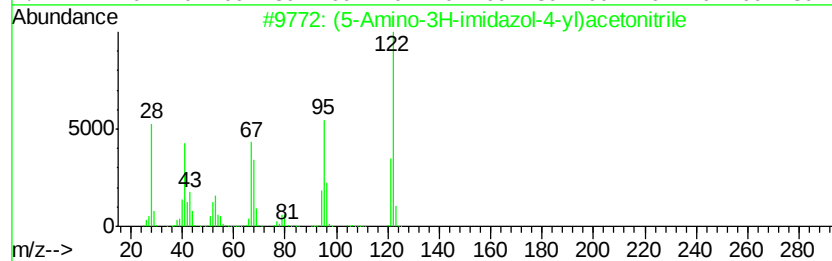
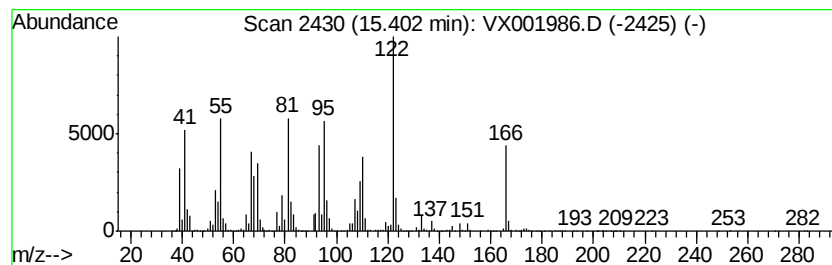
Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X052418W.M
Quant Title : SW846 8260

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

Peak Number 10 unknown15.40 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.40	19.88 ug/l	608266	1,4-Dichlorobenzene-d4	12.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(5-Amino-3H-imidazol-4-yl)aceton...	122	C5H6N4	1000191-16-3	45
2		cis,cis-1,6-Dimethylspiro[4.5]de...	166	C12H22	1000111-72-4	43
3		Naphthalene, decahydro-2,6-dimet...	166	C12H22	001618-22-0	43
4		trans, cis-3-Ethylbicyclo[4.4.0]...	166	C12H22	066660-43-3	38
5		trans,cis-1,8-Dimethylspiro[4.5]...	166	C12H22	1000111-72-9	38



Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX052518\
Data File : VX001986.D
Acq On : 25 May 2018 19:16
Operator : JC/MD
Sample : J3064-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-16

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
Sulfur dioxide	1.34	25.1	ug/l	439993	1	5.67	878314	50.0
Benzene, 1-propenyl-	12.30	29.3	ug/l	895603	4	12.09	1529600	50.0
Benzene, 2-ethyl-...	12.67	19.1	ug/l	584987	4	12.09	1529600	50.0
Indan, 1-methyl-	12.76	33.5	ug/l	1025300	4	12.09	1529600	50.0
Benzene, 1,2,3,4-...	12.98	37.3	ug/l	1140040	4	12.09	1529600	50.0
2,4-Dimethylstyrene	13.35	39.0	ug/l	1194130	4	12.09	1529600	50.0
unknown13.73	13.73	23.8	ug/l	727438	4	12.09	1529600	50.0
Benzene, (1,2-dim...	14.27	19.1	ug/l	584429	4	12.09	1529600	50.0
unknown15.40	15.40	19.9	ug/l	608266	4	12.09	1529600	50.0