LSC Area Percent Report

Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX032218\
Data File : VX000411.D
Acq On : 22 Mar 2018 17:20
Operator : JC/MD
Sample : J2005-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-1-031918

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 : W:\HPCHEM1\MSVOA_X\METHOD\82X032018W.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	89	rBV	378854	430481	6.67%	0.824%
2	1.325	109	121	143	rBV	419957	2112684	32.72%	4.043%
3	1.794	195	198	214	rVB2	39378	85830	1.33%	0.164%
4	3.074	400	408	417	rVV	85741	199622	3.09%	0.382%
5	3.215	418	431	446	rVB	220316	593831	9.20%	1.136%
6	4.403	617	626	641	rVB3	31606	94993	1.47%	0.182%
7	5.519	796	809	816	rBV2	63852	187203	2.90%	0.358%
8	5.672	828	834	840	rBV	69765	181540	2.81%	0.347%
9	5.934	867	877	891	rBV2	45815	138436	2.14%	0.265%
10	6.080	891	901	906	rVV2	67654	175216	2.71%	0.335%
11	6.153	906	913	923	rVV	221699	570050	8.83%	1.091%
12	6.269	923	932	938	rVV4	40285	137192	2.12%	0.263%
13	6.360	939	947	956	rVV3	102614	323390	5.01%	0.619%
14	6.464	957	964	978	rVB4	37622	108708	1.68%	0.208%
15	6.873	1021	1031	1039	rBV2	159815	379399	5.88%	0.726%
16	7.458	1117	1127	1139	rVB5	95319	282837	4.38%	0.541%
17	7.744	1168	1174	1185	rVB2	32581	66817	1.03%	0.128%
18	8.061	1217	1226	1239	rVB	93941	213902	3.31%	0.409%
19	8.183	1239	1246	1255	rBV2	146807	316359	4.90%	0.605%
20	8.512	1295	1300	1307	rBV4	38941	90353	1.40%	0.173%
21	8.586	1307	1312	1320	rVB4	42576	95221	1.47%	0.182%
22	8.677	1320	1327	1330	rBV3	73903	143205	2.22%	0.274%
23	8.726	1330	1335	1341	rVB	331404	529643	8.20%	1.014%
24	8.793	1341	1346	1351	rBV	178532	263971	4.09%	0.505%
25	9.031	1380	1385	1392	rVB4	65712	131204	2.03%	0.251%
26	9.122	1392	1400	1404	rVV	53457	95428	1.48%	0.183%
27	9.171	1404	1408	1413	rVB	76244	119972	1.86%	0.230%
28	9.579	1469	1475	1479	rVB4	44962	81962	1.27%	0.157%
29	10.122	1553	1564	1569	rBV	339386	492529	7.63%	0.943%
30	10.262	1581	1587	1594	rBV	3611013	4581294	70.95%	8.767%
31	10.366	1598	1604	1611	rVB	1382545	1901610	29.45%	3.639%
32	10.707	1655	1660	1672	rVB	379048	508558	7.88%	0.973%
33	11.024	1707	1712	1720	rBV	273993	368860	5.71%	0.706%
34	11.146	1725	1732	1737	rBV	321399	418631	6.48%	0.801%

LSC Area Percent Report

Data Path : W:\HPCHEM1\MSVOA X\DATA\VX032218\
Data File : VX000411.D
Acq On : 22 Mar 2018 17:20
Operator : JC/MD
Sample : J2005-06
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-1-031918

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 : W:\HPCHEM1\MSVOA_X\METHOD\82X032018W.M
Title : SW846 8260

35	11.366	1760	1768	1776	rVB	724212	918406	14.22%	1.758%
36	11.463	1776	1784	1788	rBV	386061	552855	8.56%	1.058%
37	11.677	1813	1819	1827	rBV	1537608	1853520	28.71%	3.547%
38	11.817	1837	1842	1854	rVB	5753341	6456843	100.00%	12.357%
39	11.927	1856	1860	1862	rBV	101011	125789	1.95%	0.241%
40	11.957	1862	1865	1870	rVB	125604	154861	2.40%	0.296%
41	12.085	1880	1886	1892	rVB2	466408	667740	10.34%	1.278%
42	12.152	1892	1897	1902	rBV	436194	529679	8.20%	1.014%
43	12.311	1915	1923	1929	rBV	2873531	3596470	55.70%	6.883%
44	12.378	1929	1934	1942	rVB2	796826	1157049	17.92%	2.214%
45	12.469	1944	1949	1954	rBV2	186444	250082	3.87%	0.479%
46	12.530	1954	1959	1965	rVB2	390405	548703	8.50%	1.050%
47	12.597	1965	1970	1972	rBV	1021605	1332248	20.63%	2.550%
48	12.615	1972	1973	1978	rVV	608311	593961	9.20%	1.137%
49	12.676	1978	1983	1986	rVV	1369750	1542354	23.89%	2.952%
50	12.713	1986	1989	1993	rVV	280077	350392	5.43%	0.671%
51	12.762	1993	1997	2005	rVV	825159	1330355	20.60%	2.546%
52	12.859	2009	2013	2017	rVV3	60775	98242	1.52%	0.188%
53	12.908	2017	2021	2026	rVB2	115618	170913	2.65%	0.327%
54	12.987	2026	2034	2037	rBV	1313145	1629286	25.23%	3.118%
55	13.030	2037	2041	2046	rVB	1805997	2181087	33.78%	4.174%
56	13.085	2046	2050	2058	rVB2	236022	363543	5.63%	0.696%
57	13.176	2058	2065	2067	rBV2	75507	134506	2.08%	0.257%
58	13.231	2067	2074	2078	rVV2	809512	1246171	19.30%	2.385%
59	13.274	2078	2081	2084	rVV2	103239	134206	2.08%	0.257%
60	13.317	2084	2088	2091	rVV2	236970	356777	5.53%	0.683%
61	13.359	2091	2095	2100	rVV2	1621339	2271871	35.19%	4.348%
62	13.432	2104	2107	2113	rVV	218084	292023	4.52%	0.559%
63	13.487	2113	2116	2122	rVB	156723	200999	3.11%	0.385%
64	13.566	2122	2129	2132	rBV2	158263	235954	3.65%	0.452%
65	13.609	2132	2136	2139	rVV	302137	434555	6.73%	0.832%
66	13.646	2139	2142	2149	rVV3	445911	940985	14.57%	1.801%
67	13.707	2149	2152	2153	rVV	155919	186287	2.89%	0.357%
68	13.731	2153	2156	2162	rVB3	309257	514891	7.97%	0.985%
69	13.841	2168	2174	2180	rBV	302152	425930	6.60%	0.815%
70	13.932	2184	2189	2193	rVB	127255	184932	2.86%	0.354%
71	13.993	2193	2199	2203	rBV3	149555	218117	3.38%	0.417%

LSC Area Percent Report

Data Path : W:\HPCHEM1\MSVOA X\DATA\VX032218\
Data File : VX000411.D
Acq On : 22 Mar 2018 17:20
Operator : JC/MD
Sample : J2005-06
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-1-031918

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 : W:\HPCHEM1\MSVOA_X\METHOD\82X032018W.M
Title : SW846 8260

72	14.036	2203	2206	2210	rBV	108511	120793	1.87%	0.231%
73	14.140	2219	2223	2228	rBV	186200	232999	3.61%	0.446%
74	14.280	2241	2246	2251	rBV	192682	273517	4.24%	0.523%
75	14.389	2260	2264	2268	rBV	119946	146690	2.27%	0.281%
76	14.438	2268	2272	2276	rVB	139515	166327	2.58%	0.318%
77	14.670	2304	2310	2314	rBV3	44064	82354	1.28%	0.158%
78	14.847	2334	2339	2348	rVB	491835	626967	9.71%	1.200%

Sum of corrected areas: 52253160

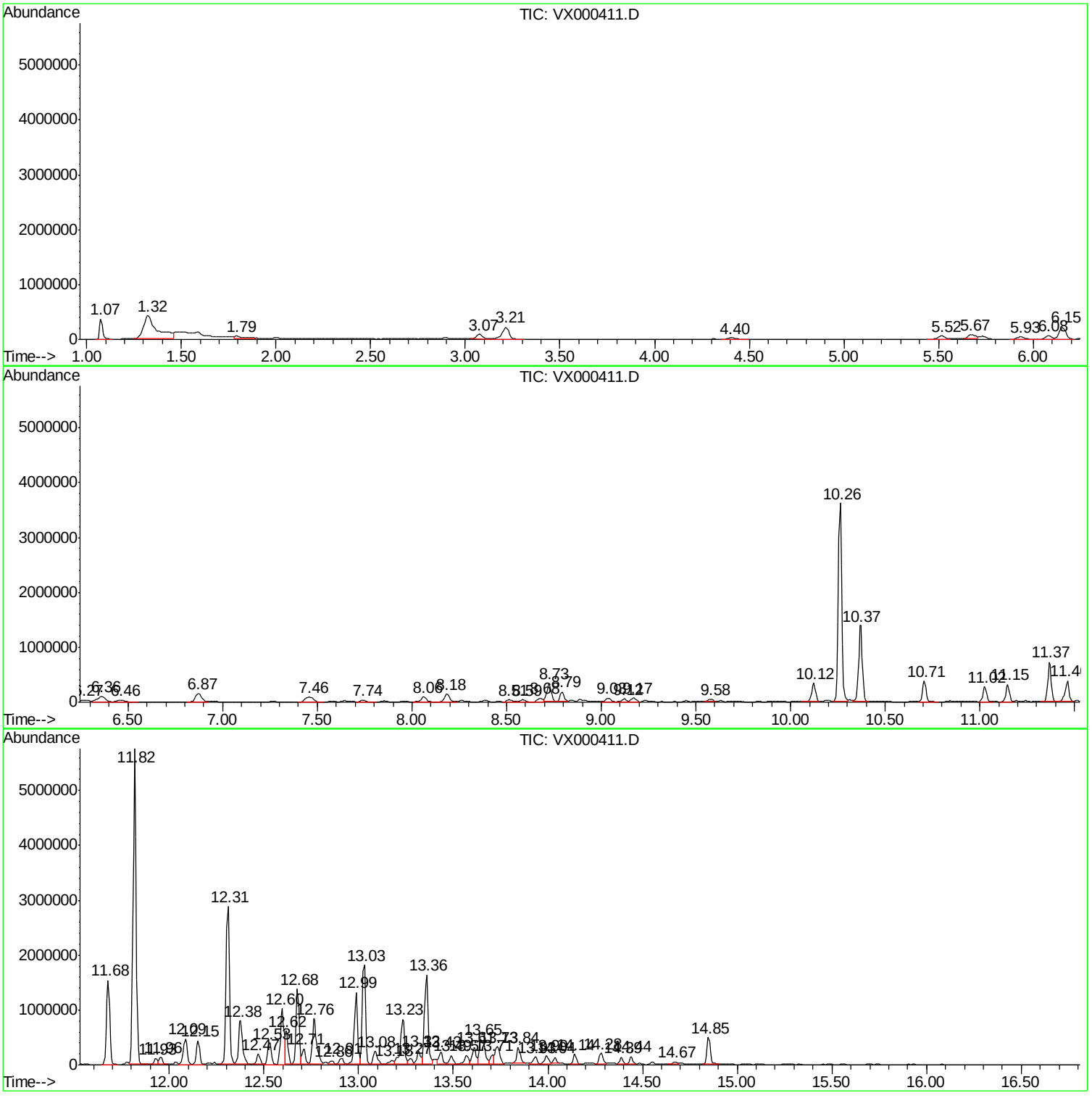
LSC Report - Integrated Chromatogram

Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX032218\
Data File : VX000411.D
Acq On : 22 Mar 2018 17:20
Operator : JC/MD
Sample : J2005-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-1-031918

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X032018W.M
Quant Title : SW846 8260

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



Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX032218\
Data File : VX000411.D
Acq On : 22 Mar 2018 17:20
Operator : JC/MD
Sample : J2005-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-1-031918

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X032018W.M
Quant Title : SW846 8260

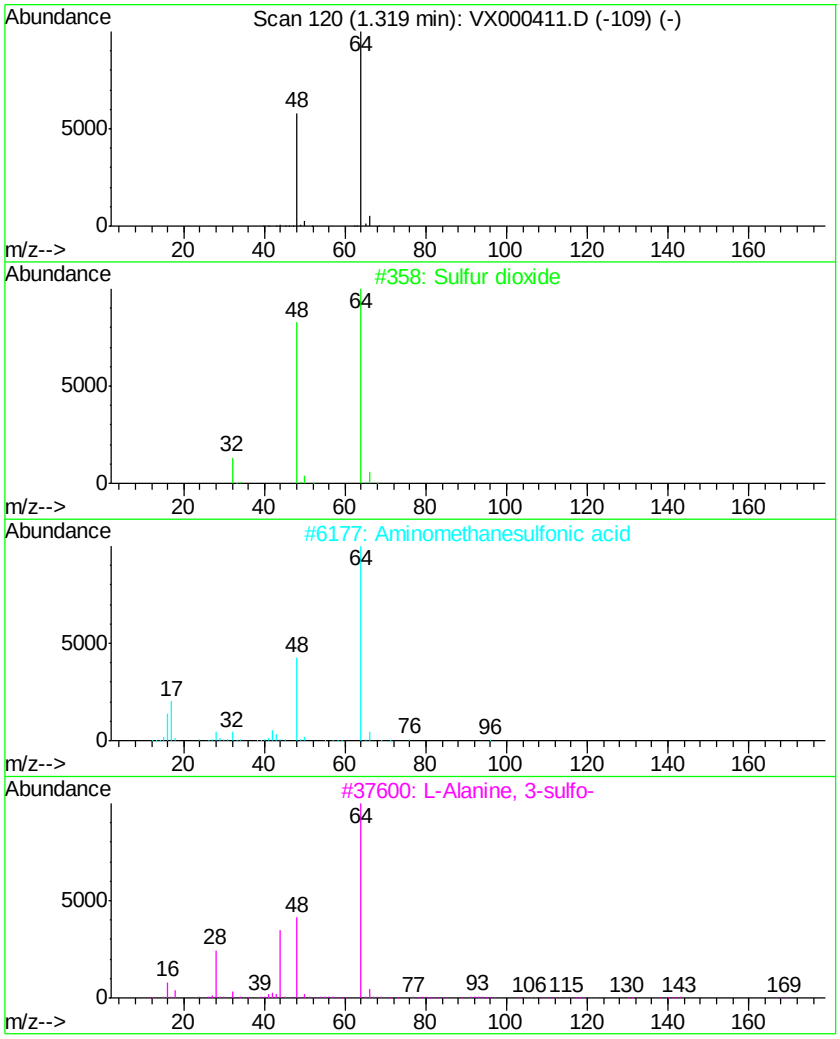
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

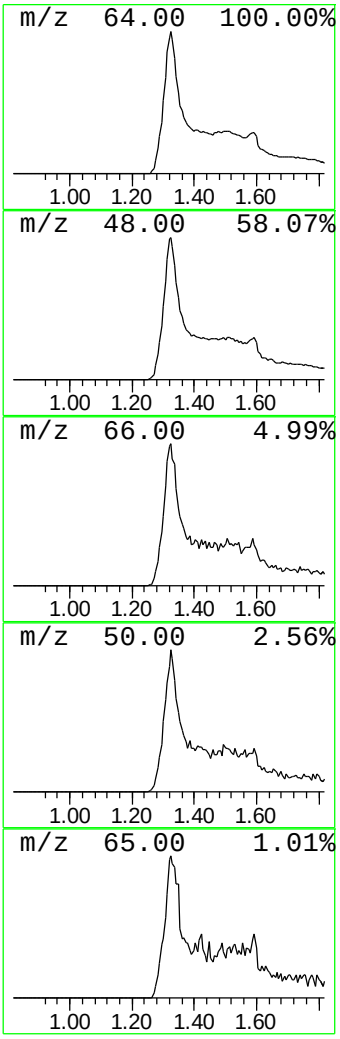
****

Peak Number 2 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.32	581.88 ug/l	2112680	Pentafluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	83
2	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
5	Ethyl Chloride	64	C2H5Cl	000075-00-3	3





Library Search Compound Report

Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX032218\
Data File : VX000411.D
Acq On : 22 Mar 2018 17:20
Operator : JC/MD
Sample : J2005-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-1-031918

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X032018W.M
Quant Title : SW846 8260

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

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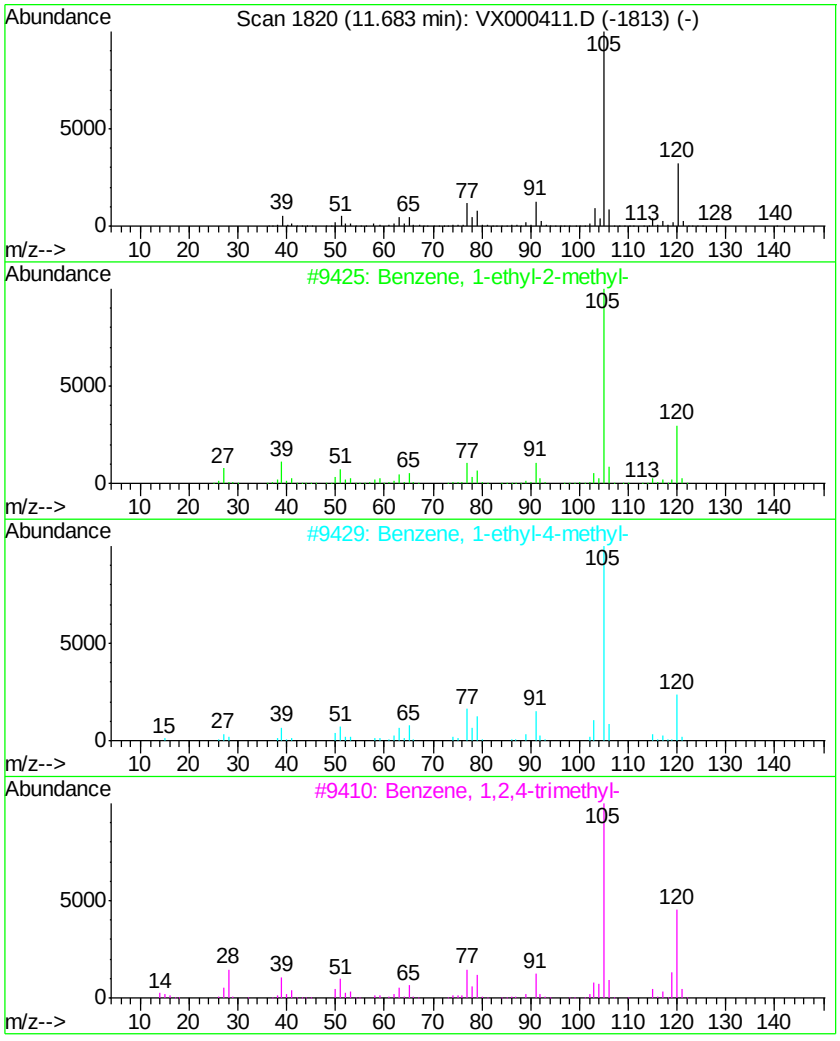
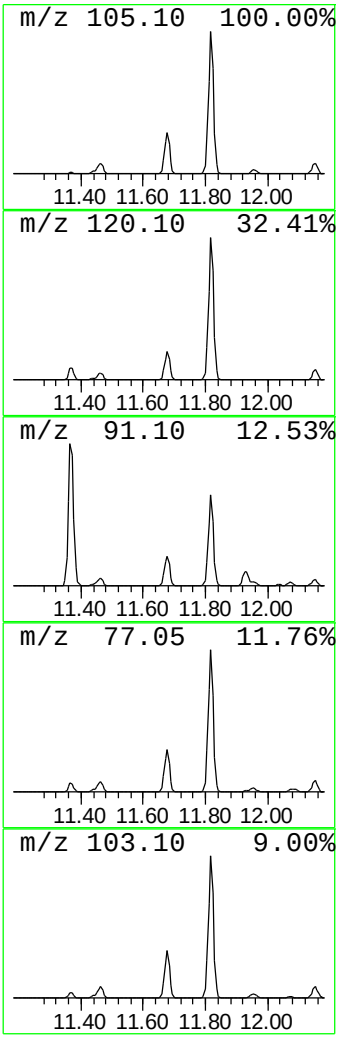
Peak Number 3 Benzene, 1-ethyl-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.68	138.79 ug/l	1853520	1,4-Dichlorobenzene-d4	12.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	93
2	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	93
3	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	90
4	Mesitylene	120	C9H12	000108-67-8	90
5	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90





Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX032218\
Data File : VX000411.D
Acq On : 22 Mar 2018 17:20
Operator : JC/MD
Sample : J2005-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-1-031918

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X032018W.M
Quant Title : SW846 8260

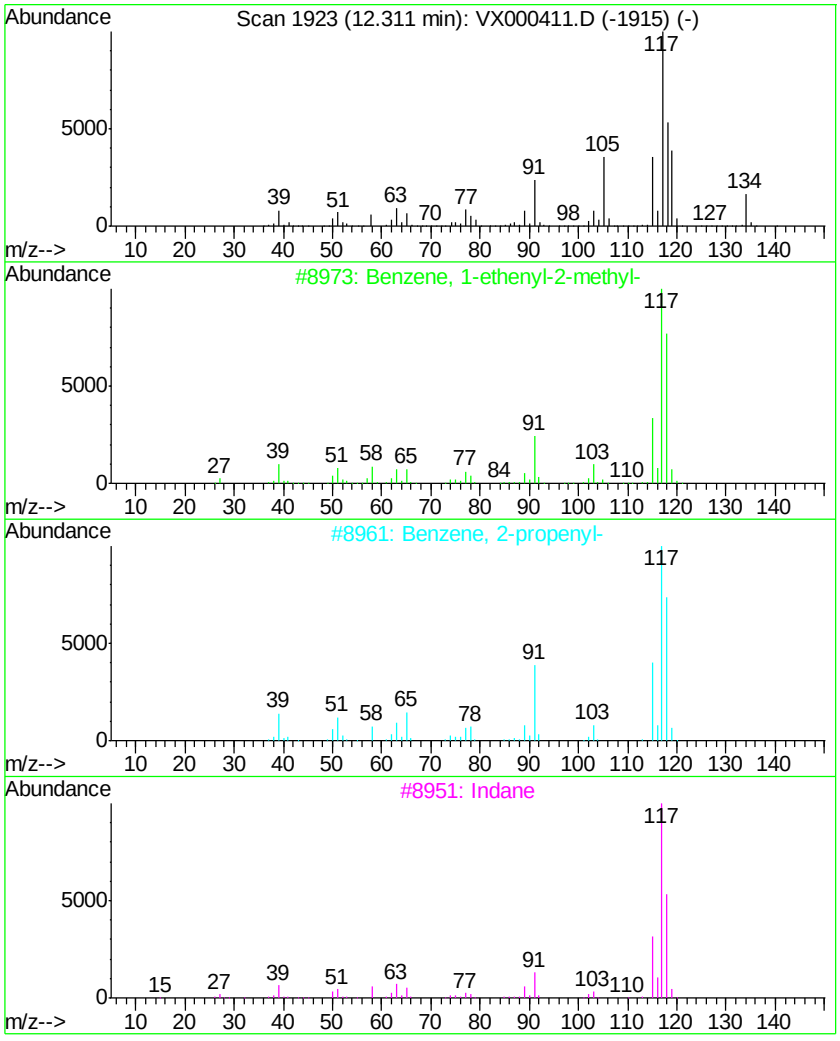
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

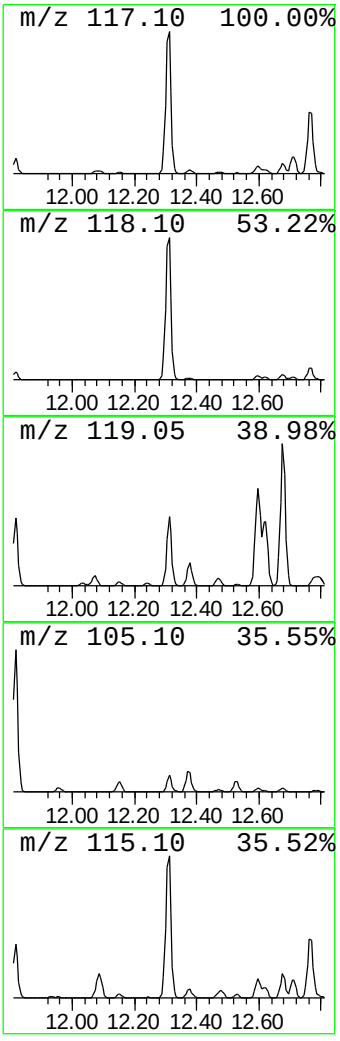
****

Peak Number 4 Benzene, 1-ethenyl-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.31	269.30 ug/l	3596470	1,4-Dichlorobenzene-d4	12.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	87
2	Benzene, 2-propenyl-	118	C9H10	000300-57-2	55
3	Indane	118	C9H10	000496-11-7	55
4	(Z)-1-Phenylpropene	118	C9H10	000766-90-5	55
5	Benzene, cyclopropyl-	118	C9H10	000873-49-4	55





Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX032218\
Data File : VX000411.D
Acq On : 22 Mar 2018 17:20
Operator : JC/MD
Sample : J2005-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-1-031918

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X032018W.M
Quant Title : SW846 8260

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

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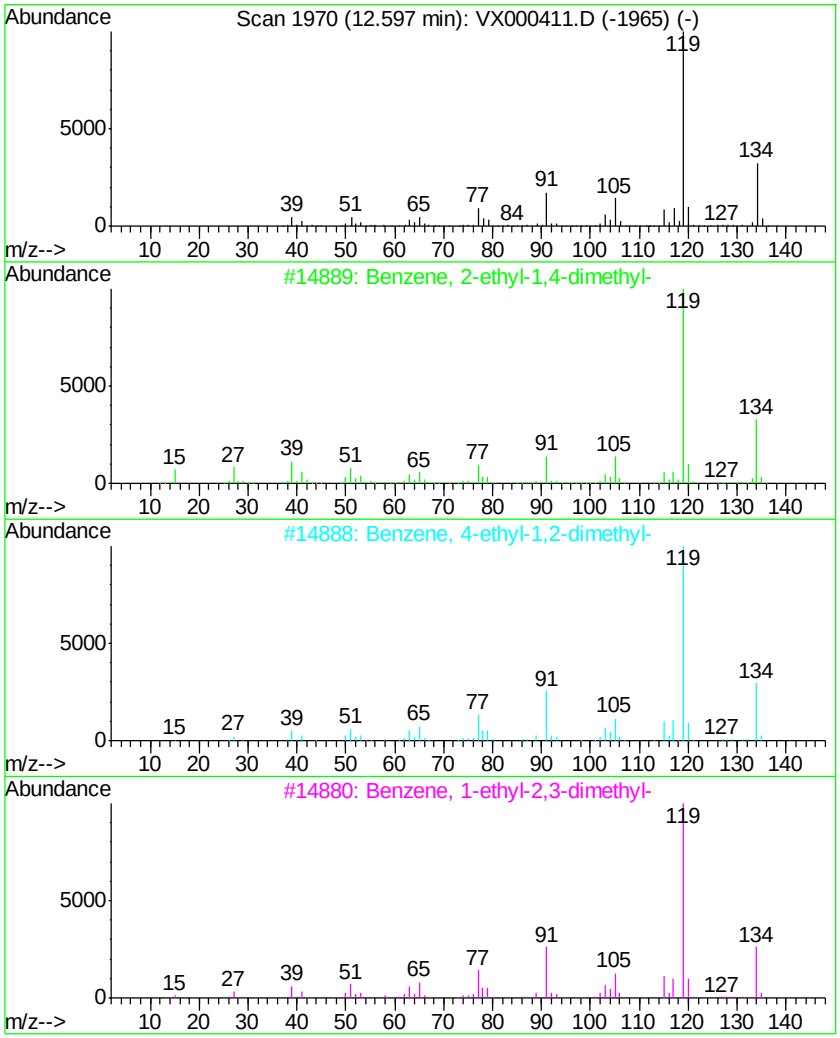
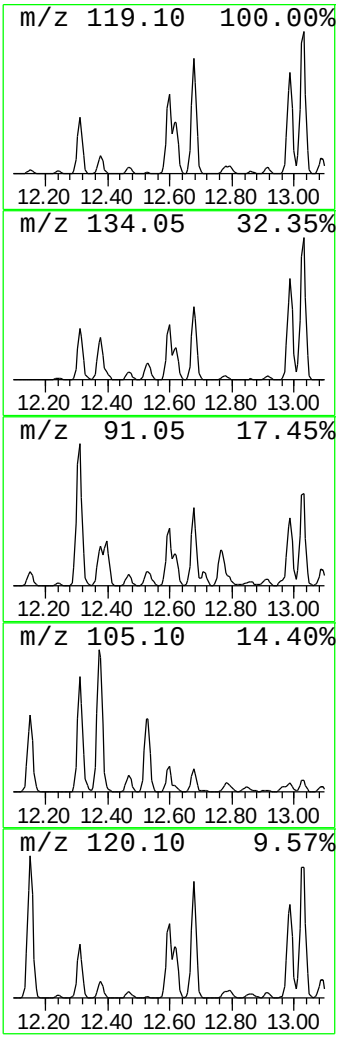
Peak Number 5 Benzene, 2-ethyl-1,4-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.60	99.76 ug/l	1332250	1,4-Dichlorobenzene-d4	12.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	97
2	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	95
3	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95
4	o-Cymene	134	C10H14	000527-84-4	94
5	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	93





Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX032218\
Data File : VX000411.D
Acq On : 22 Mar 2018 17:20
Operator : JC/MD
Sample : J2005-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-1-031918

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X032018W.M
Quant Title : SW846 8260

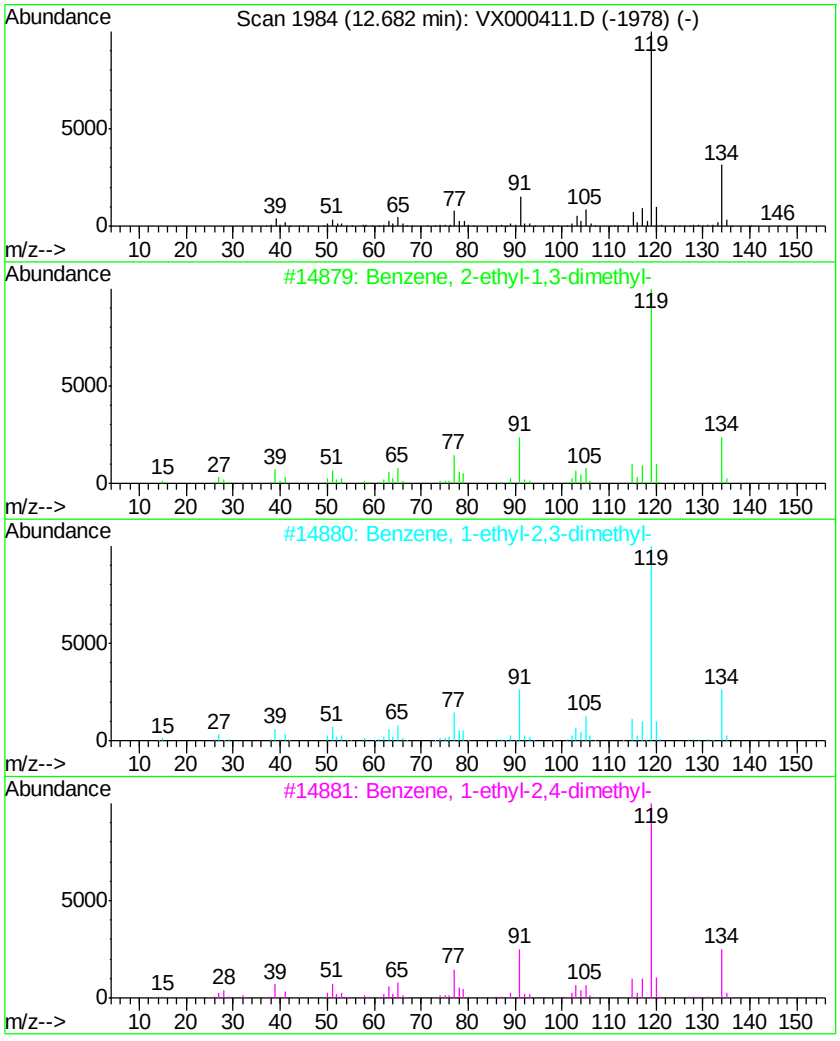
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

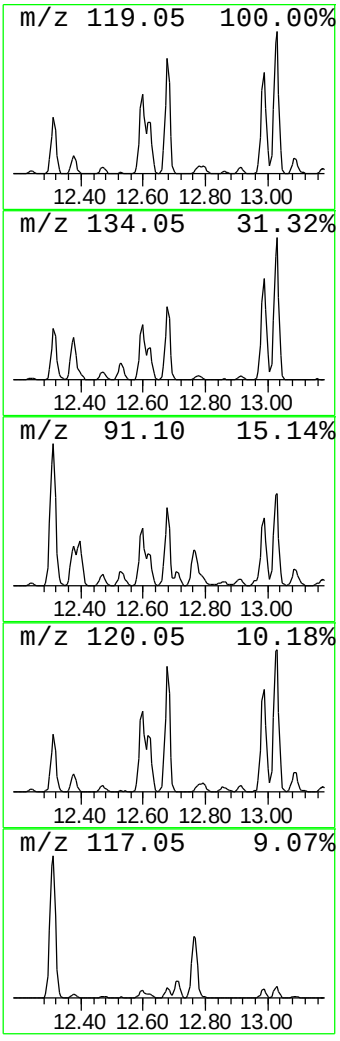
****

Peak Number 6 Benzene, 2-ethyl-1,3-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.68	115.49 ug/l	1542350	1,4-Dichlorobenzene-d4	12.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	95
2	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95
3	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	95
4	o-Cymene	134	C10H14	000527-84-4	95
5	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	95





Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX032218\
Data File : VX000411.D
Acq On : 22 Mar 2018 17:20
Operator : JC/MD
Sample : J2005-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-1-031918

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X032018W.M
Quant Title : SW846 8260

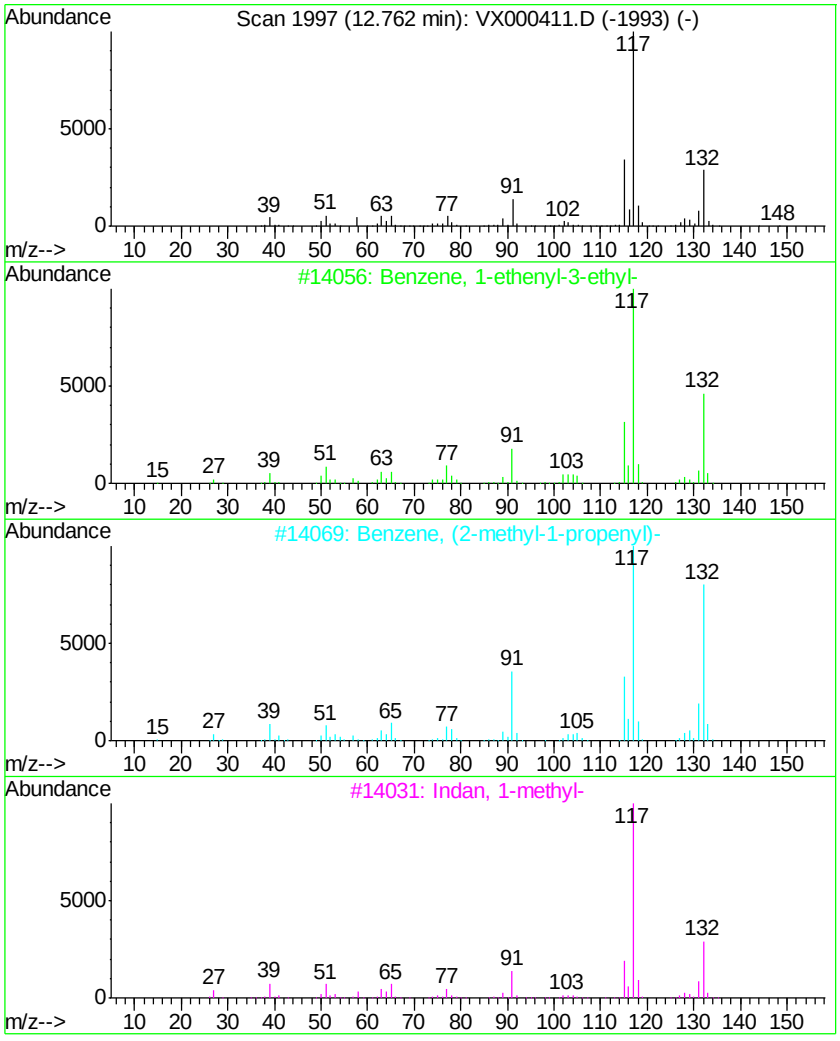
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

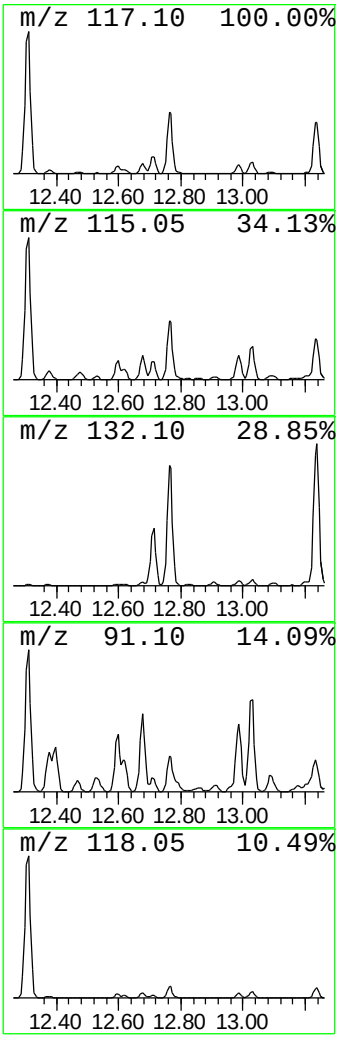
****

Peak Number 7 Benzene, 1-ethenyl-3-ethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.76	99.62 ug/l	1330360	1,4-Dichlorobenzene-d4	12.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	91
2	Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	87
3	Indan, 1-methyl-	132	C10H12	000767-58-8	87
4	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	86
5	Benzene, (2-methylcyclopropyl)-	132	C10H12	1000327-39-0	86





Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX032218\
Data File : VX000411.D
Acq On : 22 Mar 2018 17:20
Operator : JC/MD
Sample : J2005-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-1-031918

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X032018W.M
Quant Title : SW846 8260

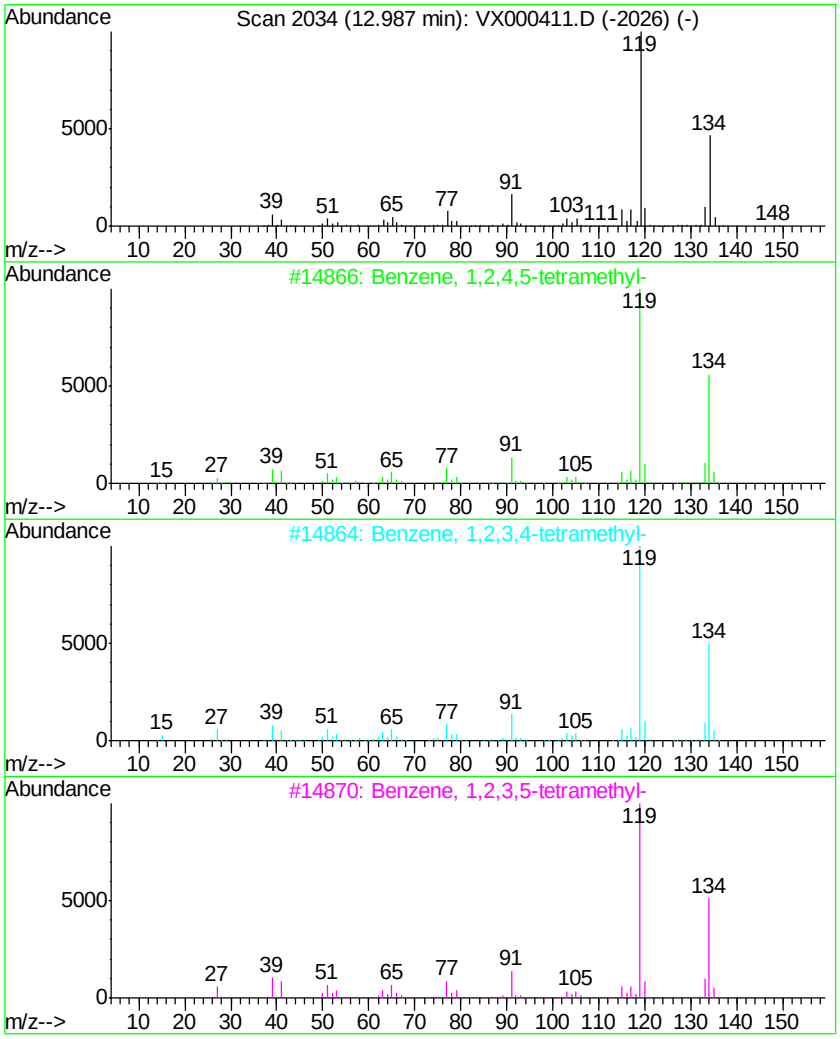
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

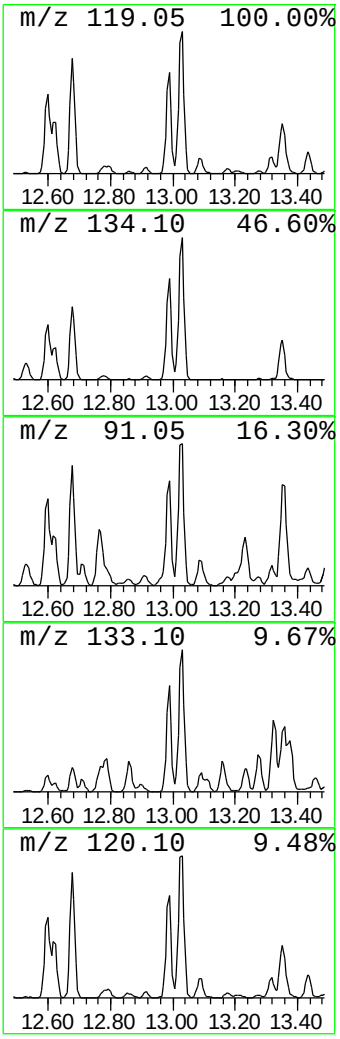
****

Peak Number 8 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.99	122.00 ug/l	1629290	1,4-Dichlorobenzene-d4	12.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	97
2	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	97
3	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	95
4	o-Cymene	134	C10H14	000527-84-4	95
5	1,3-Cyclopentadiene, 1,2,3,4-tet...	134	C10H14	076089-59-3	94





Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX032218\
Data File : VX000411.D
Acq On : 22 Mar 2018 17:20
Operator : JC/MD
Sample : J2005-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-1-031918

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X032018W.M
Quant Title : SW846 8260

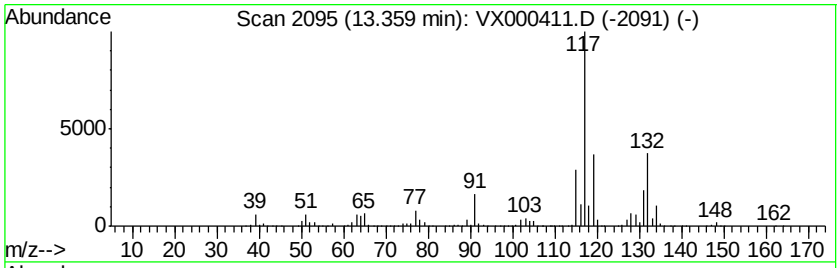
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

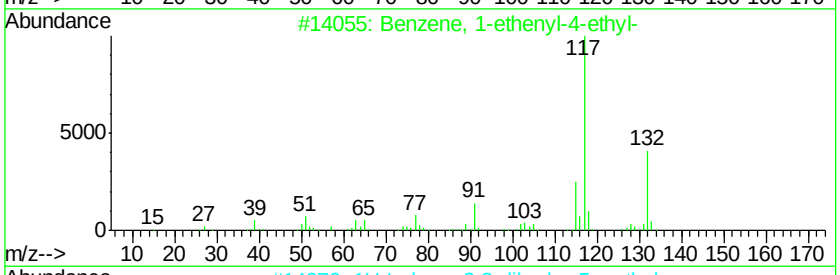
****

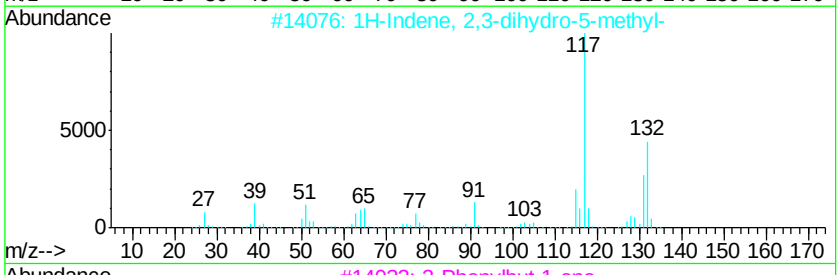
Peak Number 10 Benzene, 1-ethenyl-4-ethyl- Concentration Rank 3

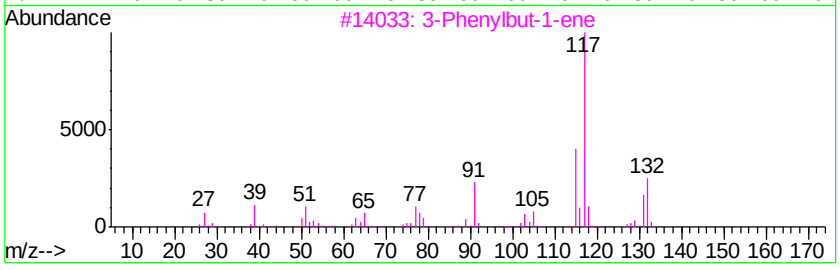
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.36	170.12 ug/l	2271870	1,4-Dichlorobenzene-d4	12.09

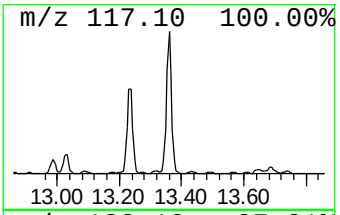
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
2	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	89
3	3-Phenylbut-1-ene	132	C10H12	000934-10-1	87
4	Benzene, 2-butenyl-	132	C10H12	001560-06-1	87
5	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	83

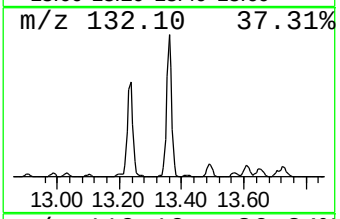


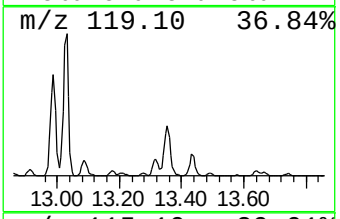


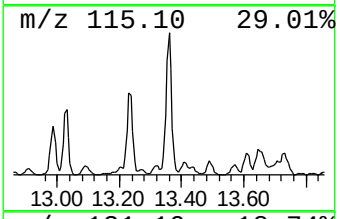


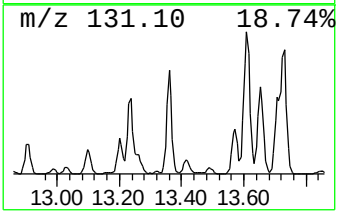












Tentatively Identified Compound (LSC) summary

Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX032218\
Data File : VX000411.D
Acq On : 22 Mar 2018 17:20
Operator : JC/MD
Sample : J2005-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-1-031918

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X032018W.M
Quant Title : SW846 8260

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Sulfur dioxide	1.32	581.9	ug/l	2112680	1	5.67	181540	50.0
Benzene, 1-ethyl-...	11.68	138.8	ug/l	1853520	4	12.09	667740	50.0
Benzene, 1-etheny...	12.31	269.3	ug/l	3596470	4	12.09	667740	50.0
Benzene, 2-ethyl-...	12.60	99.8	ug/l	1332250	4	12.09	667740	50.0
Benzene, 2-ethyl-...	12.68	115.5	ug/l	1542350	4	12.09	667740	50.0
Benzene, 1-etheny...	12.76	99.6	ug/l	1330360	4	12.09	667740	50.0
Benzene, 1,2,4,5-...	12.99	122.0	ug/l	1629290	4	12.09	667740	50.0
Benzene, 1-etheny...	13.36	170.1	ug/l	2271870	4	12.09	667740	50.0