LSC Area Percent Report

Data Path : W:\HPCHEM1\MSVOA X\DATA\VX032218\
Data File : VX000413.D
Acq On : 22 Mar 2018 18:11
Operator : JC/MD
Sample : J2005-08
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-7-031918

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	94	rBV	416389	464218	84.70%	8.501%
2	1.276	109	113	120	rBV	43170	62745	11.45%	1.149%
3	1.593	159	165	170	rBV2	6211	9816	1.79%	0.180%
4	1.794	193	198	205	rVB	29398	39344	7.18%	0.721%
5	2.398	290	297	303	rBV3	6872	15189	2.77%	0.278%
6	2.849	364	371	377	rBV3	9174	23410	4.27%	0.429%
7	2.934	380	385	399	rVB2	13353	33004	6.02%	0.604%
8	3.172	417	424	427	rBV5	6803	14853	2.71%	0.272%
9	4.312	603	611	613	rBV4	2939	6578	1.20%	0.120%
10	4.416	620	628	637	rVB4	6629	18198	3.32%	0.333%
11	5.513	797	808	825	rBV2	67015	199493	36.40%	3.653%
12	5.672	825	834	858	rVB2	97479	301814	55.07%	5.527%
13	6.080	890	901	910	rBV	76191	193747	35.35%	3.548%
14	6.153	910	913	922	rVB3	5910	12673	2.31%	0.232%
15	6.354	937	946	954	rVV2	11137	31113	5.68%	0.570%
16	6.458	958	963	974	rVB6	2593	6609	1.21%	0.121%
17	6.873	1021	1031	1041	rBV	164689	390110	71.18%	7.144%
18	7.452	1118	1126	1134	rVB4	5693	13438	2.45%	0.246%
19	7.854	1186	1192	1200	rBV5	3084	6896	1.26%	0.126%
20	8.067	1220	1227	1234	rVB3	10647	23209	4.23%	0.425%
21	8.183	1237	1246	1256	rBV2	21532	43320	7.90%	0.793%
22	8.592	1306	1313	1320	rVB6	3443	7056	1.29%	0.129%
23	8.726	1328	1335	1343	rVB	353966	548068	100.00%	10.037%
24	9.031	1379	1385	1393	rVB	88048	136784	24.96%	2.505%
25	9.122	1393	1400	1405	rVV	82525	123399	22.52%	2.260%
26	9.171	1405	1408	1413	rVB3	6379	9422	1.72%	0.173%
27	9.573	1470	1474	1482	rVB5	3866	6102	1.11%	0.112%
28	10.122	1555	1564	1573	rBV	377508	504430	92.04%	9.238%
29	10.189	1573	1575	1583	rVB5	3200	5942	1.08%	0.109%
30	10.262	1583	1587	1592	rBV	16072	21739	3.97%	0.398%
31	11.024	1707	1712	1717	rBV	63111	82199	15.00%	1.505%
32	11.146	1725	1732	1738	rBV	304535	378872	69.13%	6.938%
33	11.366	1764	1768	1773	rVB	31213	38461	7.02%	0.704%
34	11.927	1854	1860	1862	rBV	13590	17025	3.11%	0.312%

LSC Area Percent Report

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Data File : VX000413.D
Acq On : 22 Mar 2018 18:11
Operator : JC/MD
Sample : J2005-08
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-7-031918

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	11.957	1862	1865	1869	rVB2	18755	23698	4.32%	0.434%
36	12.085	1881	1886	1894	rVB	377884	456165	83.23%	8.354%
37	12.244	1908	1912	1915	rVB	6023	7274	1.33%	0.133%
38	12.311	1915	1923	1929	rVV	307843	379586	69.26%	6.951%
39	12.378	1929	1934	1942	rVB	46606	57972	10.58%	1.062%
40	12.469	1944	1949	1954	rBV3	14166	17718	3.23%	0.324%
41	12.536	1954	1960	1965	rBV2	18353	25735	4.70%	0.471%
42	12.676	1975	1983	1986	rBV	75743	89469	16.32%	1.638%
43	12.707	1986	1988	1993	rVV	37144	46032	8.40%	0.843%
44	12.762	1993	1997	2004	rVV	144051	186195	33.97%	3.410%
45	12.823	2004	2007	2011	rVV2	4826	5784	1.06%	0.106%
46	12.902	2015	2020	2025	rBV2	11127	16041	2.93%	0.294%
47	12.987	2025	2034	2038	rBV	51211	65190	11.89%	1.194%
48	13.091	2046	2051	2058	rVB3	16809	26877	4.90%	0.492%
49	13.201	2064	2069	2071	rBV3	11006	11377	2.08%	0.208%
50	13.237	2071	2075	2078	rBV	34696	41615	7.59%	0.762%
51	13.323	2083	2089	2093	rBV5	6006	10065	1.84%	0.184%
52	13.414	2100	2104	2106	rBV2	6055	8204	1.50%	0.150%
53	13.573	2123	2130	2132	rBV4	6526	8417	1.54%	0.154%
54	13.609	2132	2136	2139	rVV	23002	32606	5.95%	0.597%
55	13.646	2139	2142	2146	rVV4	15238	22265	4.06%	0.408%
56	13.707	2146	2152	2153	rVV2	24019	36891	6.73%	0.676%
57	13.731	2153	2156	2162	rVB2	38833	52499	9.58%	0.961%
58	13.987	2191	2198	2203	rBV	11955	16207	2.96%	0.297%
59	14.140	2219	2223	2227	rBV	8643	10826	1.98%	0.198%
60	14.280	2240	2246	2250	rBV4	6296	9030	1.65%	0.165%
61	14.438	2268	2272	2276	rBV3	5891	7597	1.39%	0.139%

Sum of corrected areas: 5460611

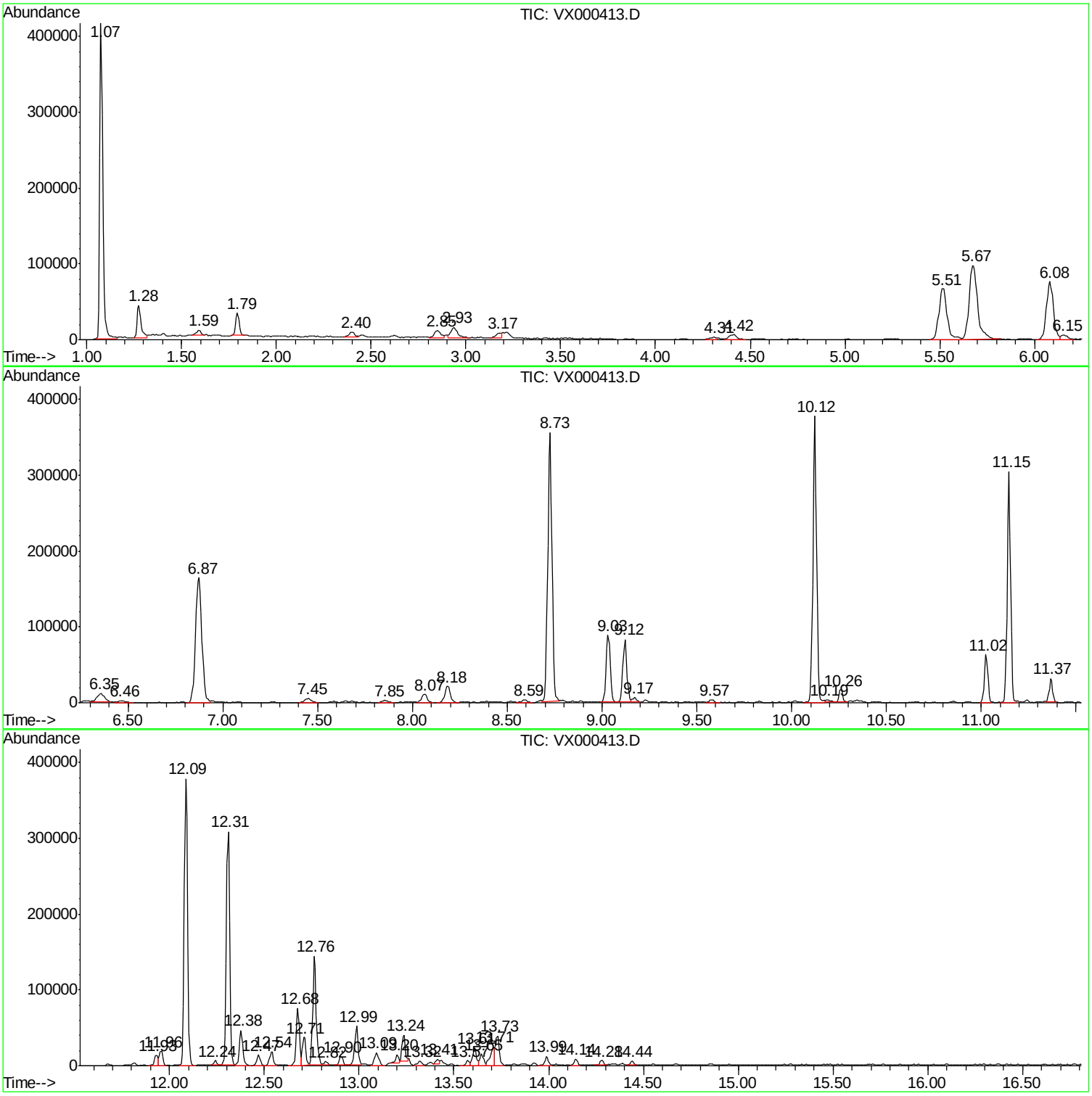
LSC Report - Integrated Chromatogram

Data Path : W:\HPCHEM1\MSVOA X\DATA\VX032218\
Data File : VX000413.D
Acq On : 22 Mar 2018 18:11
Operator : JC/MD
Sample : J2005-08
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-7-031918

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

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



Library Search Compound Report

Data Path : W:\HPCHEM1\MSVOA X\DATA\VX032218\
Data File : VX000413.D
Acq On : 22 Mar 2018 18:11
Operator : JC/MD
Sample : J2005-08
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-7-031918

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

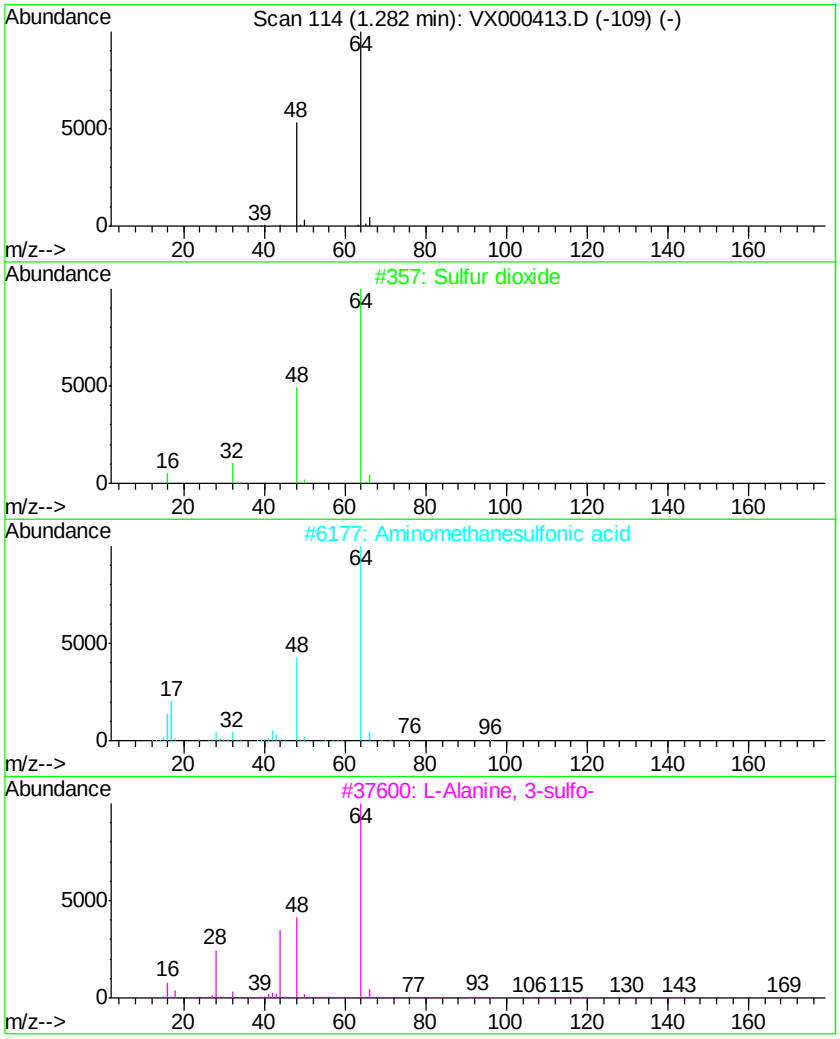
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

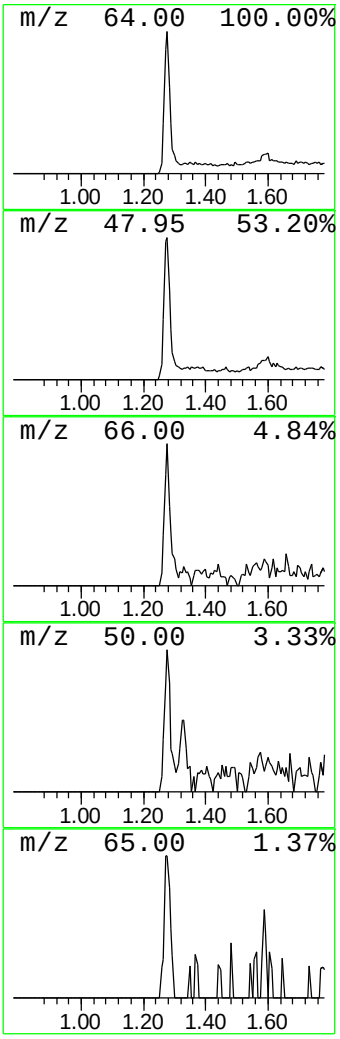
****

Peak Number 2 Sulfur dioxide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.28	10.39 ug/l	62745	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 : VX000413.D
Acq On : 22 Mar 2018 18:11
Operator : JC/MD
Sample : J2005-08
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-7-031918

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

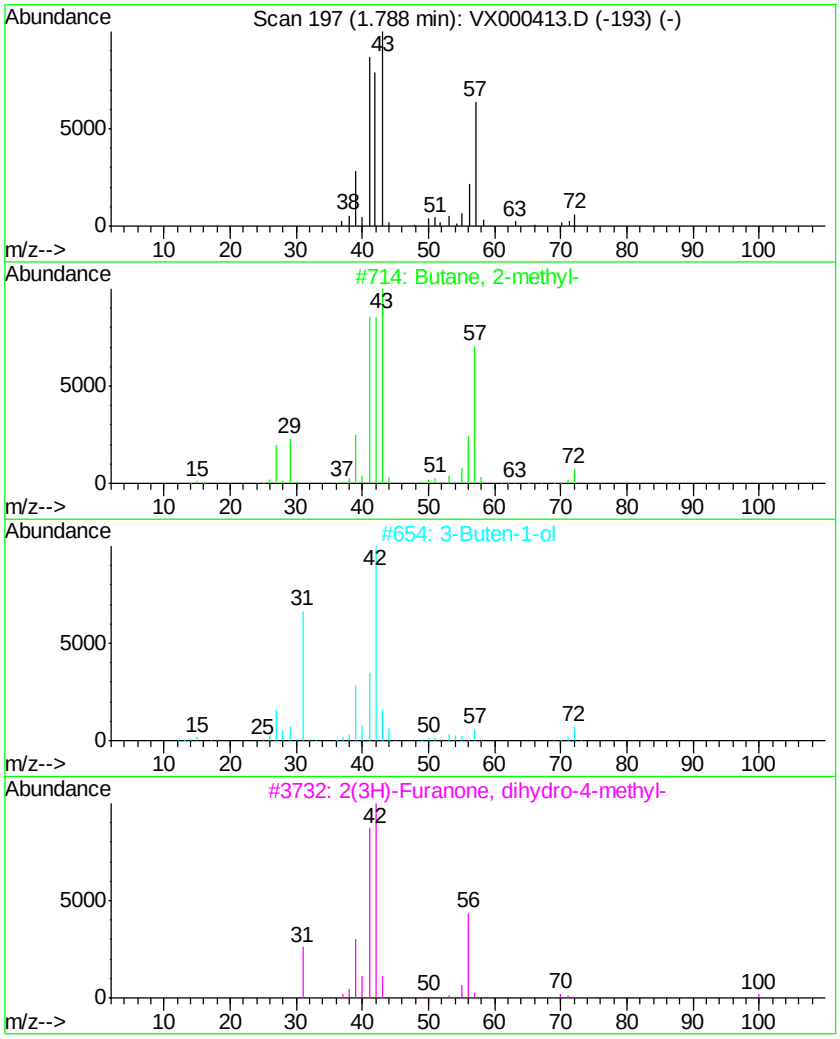
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

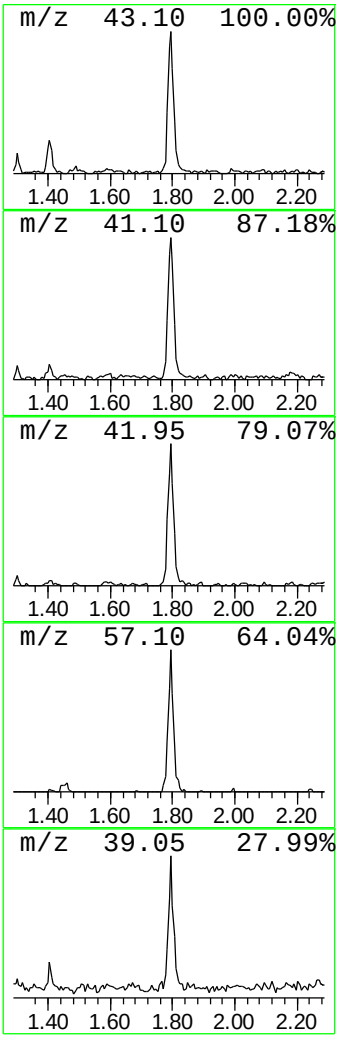
****

Peak Number 3 Butane, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.79	6.52 ug/l	39344	Pentafluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	91
2	3-Buten-1-ol	72	C4H8O	000627-27-0	43
3	2(3H)-Furanone, dihydro-4-methyl-	100	C5H8O2	001679-49-8	42
4	Pentane	72	C5H12	000109-66-0	33
5	Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	16





Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX032218\
Data File : VX000413.D
Acq On : 22 Mar 2018 18:11
Operator : JC/MD
Sample : J2005-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-7-031918

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

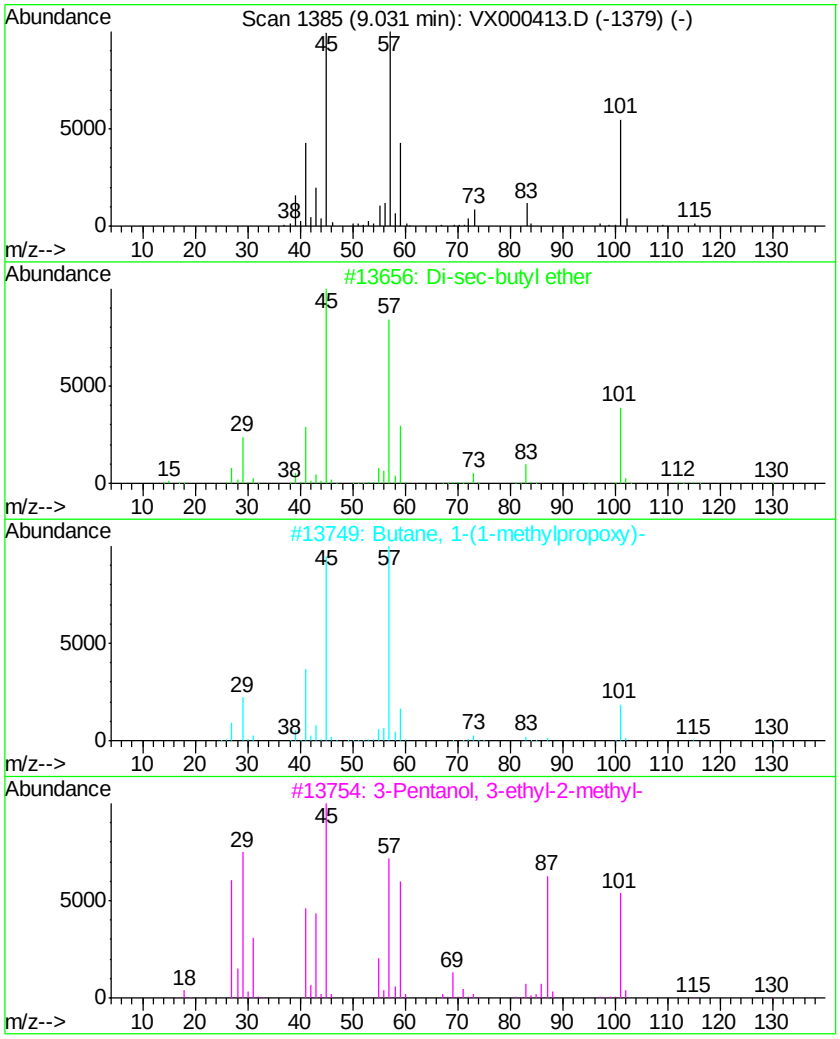
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

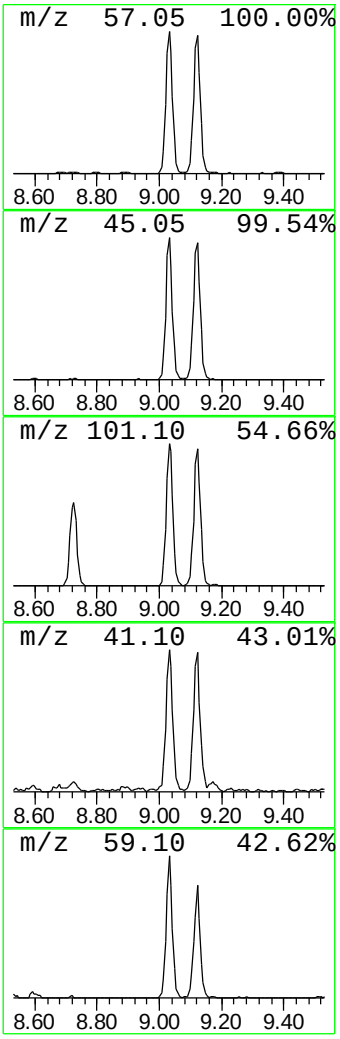
****

Peak Number 4 Di-sec-butyl ether Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.03	13.56 ug/l	136784	Chlorobenzene-d5	10.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Di-sec-butyl ether	130	C8H18O	006863-58-7	90
2	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	64
3	3-Pentanol, 3-ethyl-2-methyl-	130	C8H18O	000597-05-7	64
4	Sulfurous acid, isobutyl 2-methy...	238	C10H22O4S	1000309-20-3	50
5	Butanoic acid, 4-methoxy-	118	C5H10O3	029006-02-8	47





Library Search Compound Report

Data Path : W:\HPCHEM1\MSVOA X\DATA\VX032218\
Data File : VX000413.D
Acq On : 22 Mar 2018 18:11
Operator : JC/MD
Sample : J2005-08
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-7-031918

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

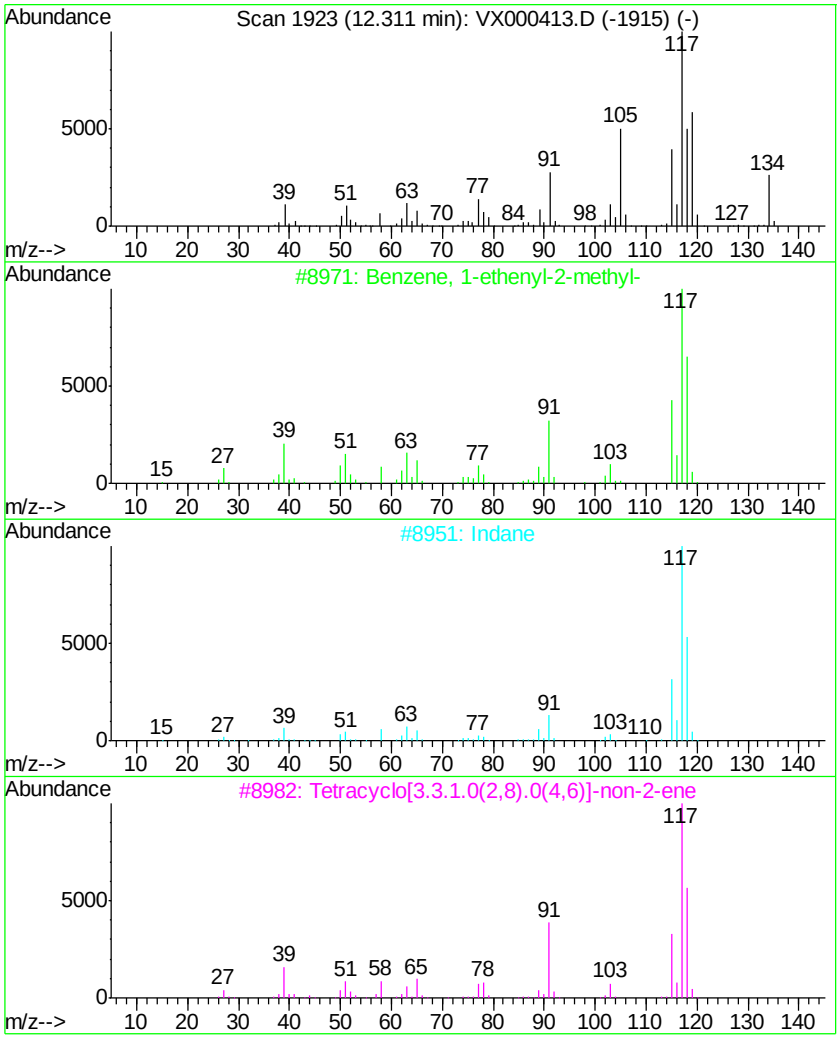
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

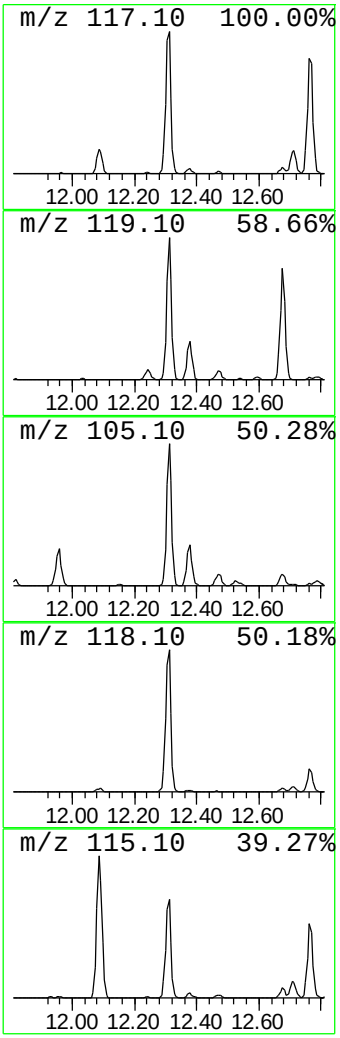
****

Peak Number 6 Benzene, 1-ethenyl-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.31	41.61 ug/l	379586	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	80
2	Indane	118	C9H10	000496-11-7	55
3	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	55
4	Deltacyclene	118	C9H10	007785-10-6	55
5	Benzene, cyclopropyl-	118	C9H10	000873-49-4	50





Library Search Compound Report

Data Path : W:\HPCHEM1\MSVOA X\DATA\VX032218\
Data File : VX000413.D
Acq On : 22 Mar 2018 18:11
Operator : JC/MD
Sample : J2005-08
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-7-031918

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

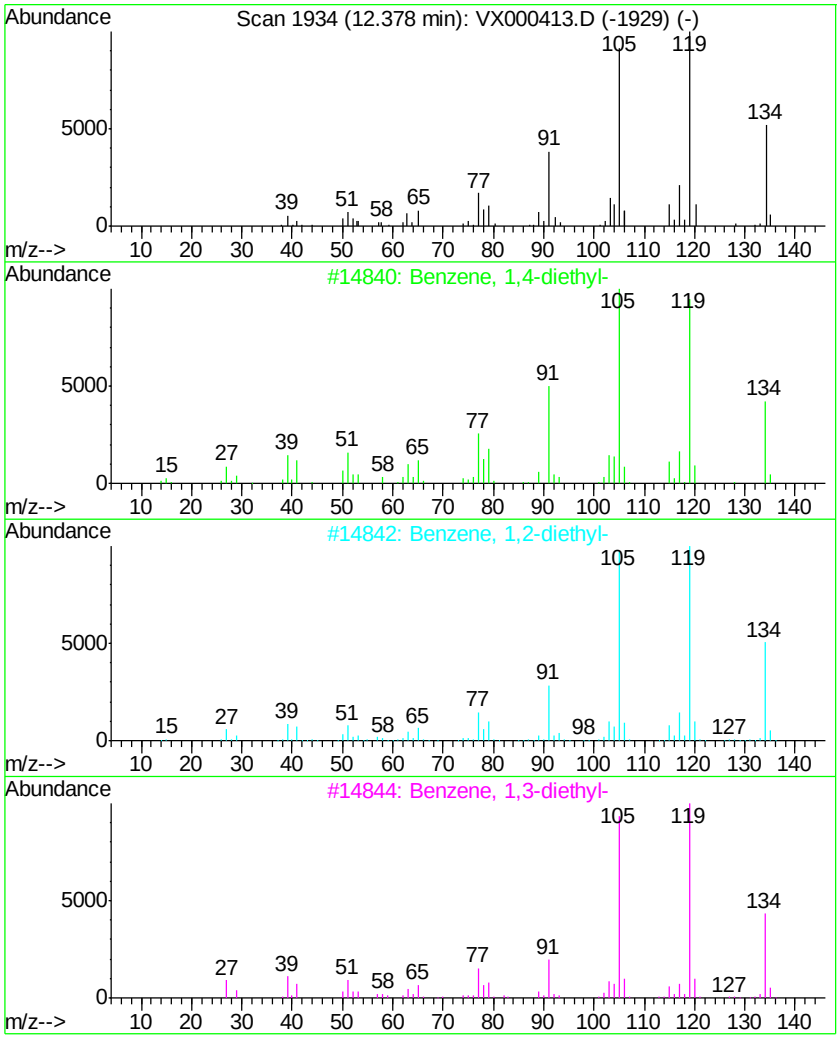
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

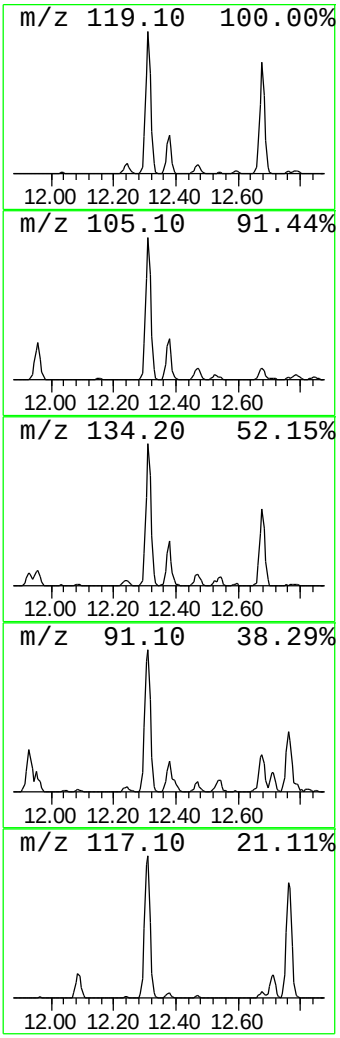
****

Peak Number 7 Benzene, 1,4-diethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.38	6.35 ug/l	57972	1,4-Dichlorobenzene-d4	12.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,4-diethyl-	134	C10H14	000105-05-5	97
2	Benzene, 1,2-diethyl-	134	C10H14	000135-01-3	95
3	Benzene, 1,3-diethyl-	134	C10H14	000141-93-5	90
4	Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	87
5	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	87





Library Search Compound Report

Data Path : W:\HPCHEM1\MSVOA X\DATA\VX032218\
Data File : VX000413.D
Acq On : 22 Mar 2018 18:11
Operator : JC/MD
Sample : J2005-08
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-7-031918

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

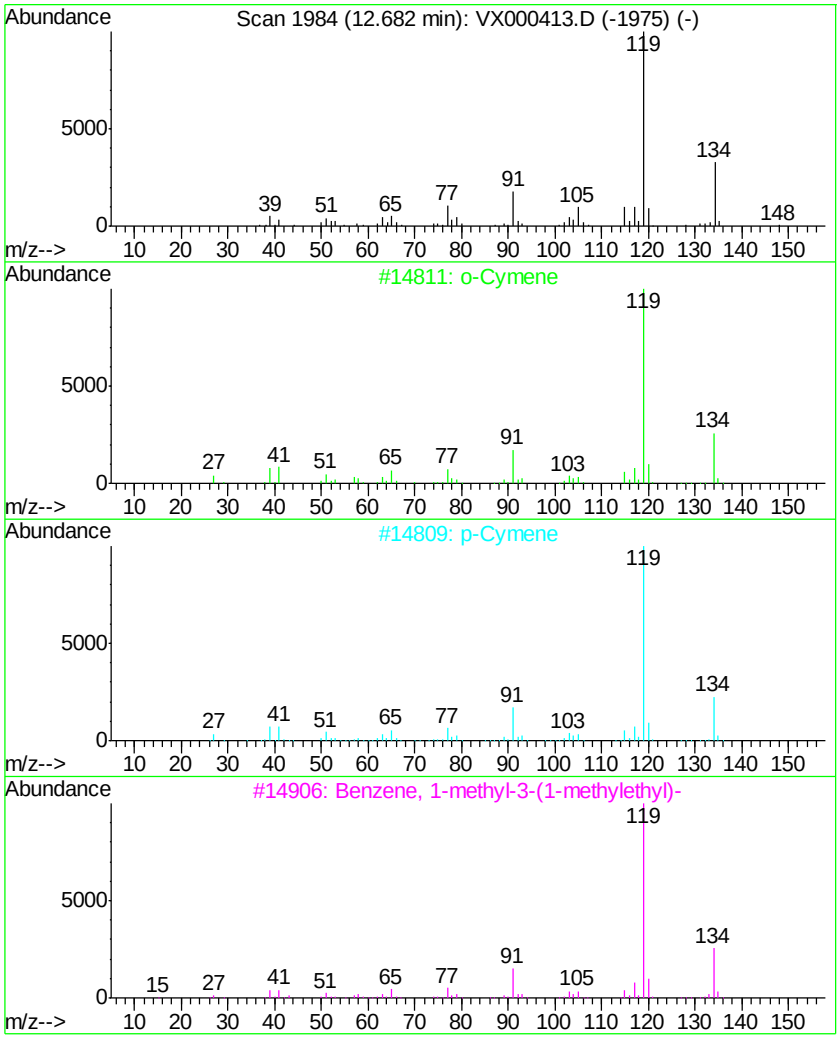
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

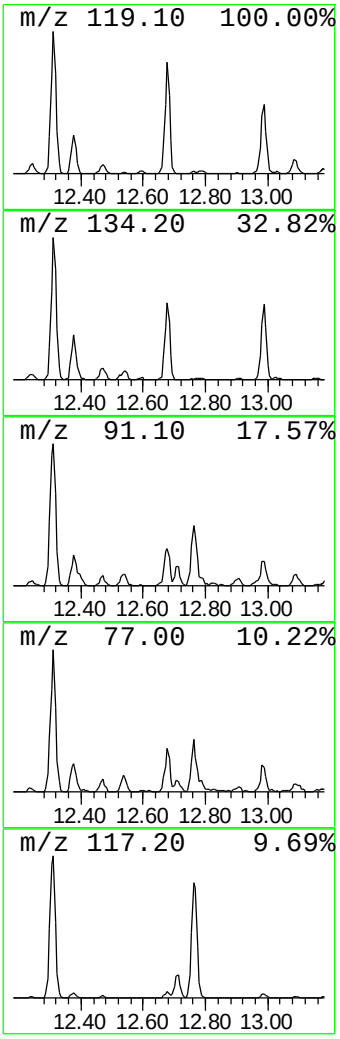
****

Peak Number 8 o-Cymene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.68	9.81 ug/l	89469	1,4-Dichlorobenzene-d4	12.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	o-Cymene	134	C10H14	000527-84-4	97
2	p-Cymene	134	C10H14	000099-87-6	97
3	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	95
4	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95
5	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	94





Library Search Compound Report

Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX032218\
Data File : VX000413.D
Acq On : 22 Mar 2018 18:11
Operator : JC/MD
Sample : J2005-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-7-031918

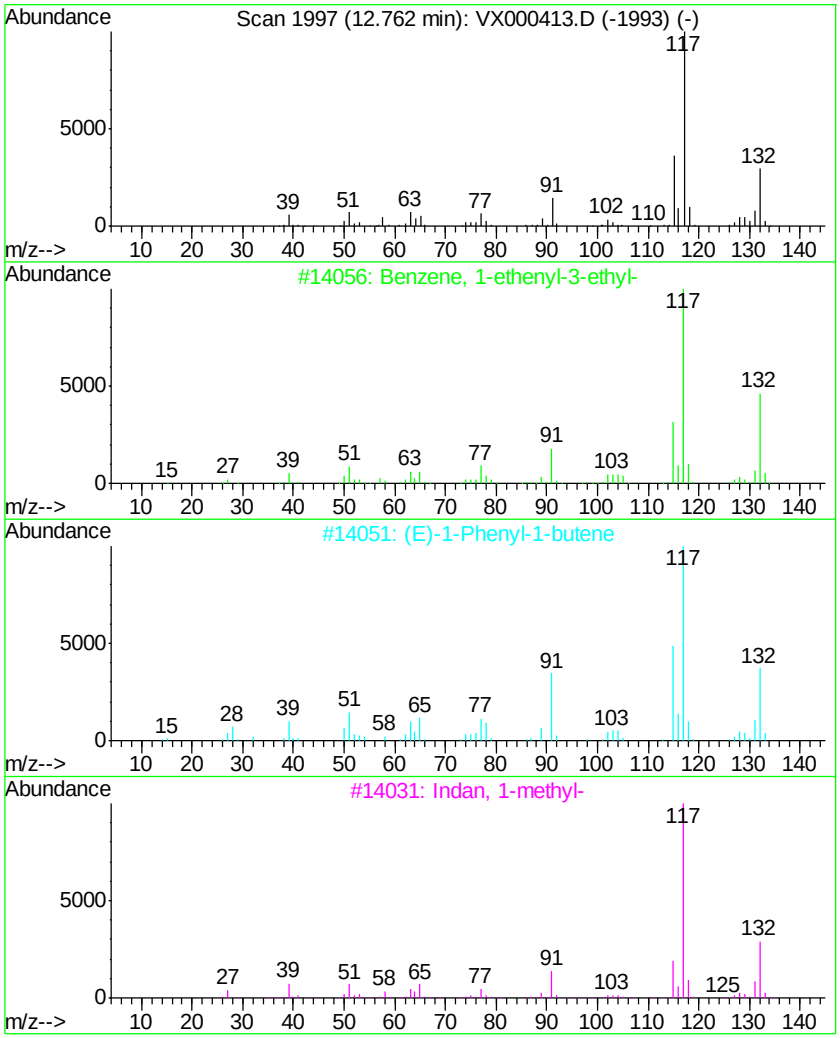
Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X032018W.M
Quant Title : SW846 8260

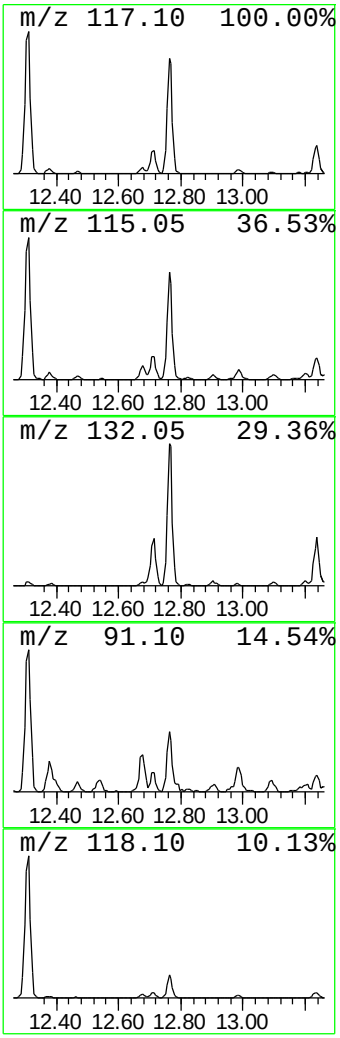
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, 1-ethenyl-3-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.76	20.41 ug/l	186195	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	(E)-1-Phenyl-1-butene	132	C10H12	001005-64-7	87
3	Indan, 1-methyl-	132	C10H12	000767-58-8	87
4	Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	83
5	3-Phenylbut-1-ene	132	C10H12	000934-10-1	83





Library Search Compound Report

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Data File : VX000413.D
Acq On : 22 Mar 2018 18:11
Operator : JC/MD
Sample : J2005-08
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-7-031918

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

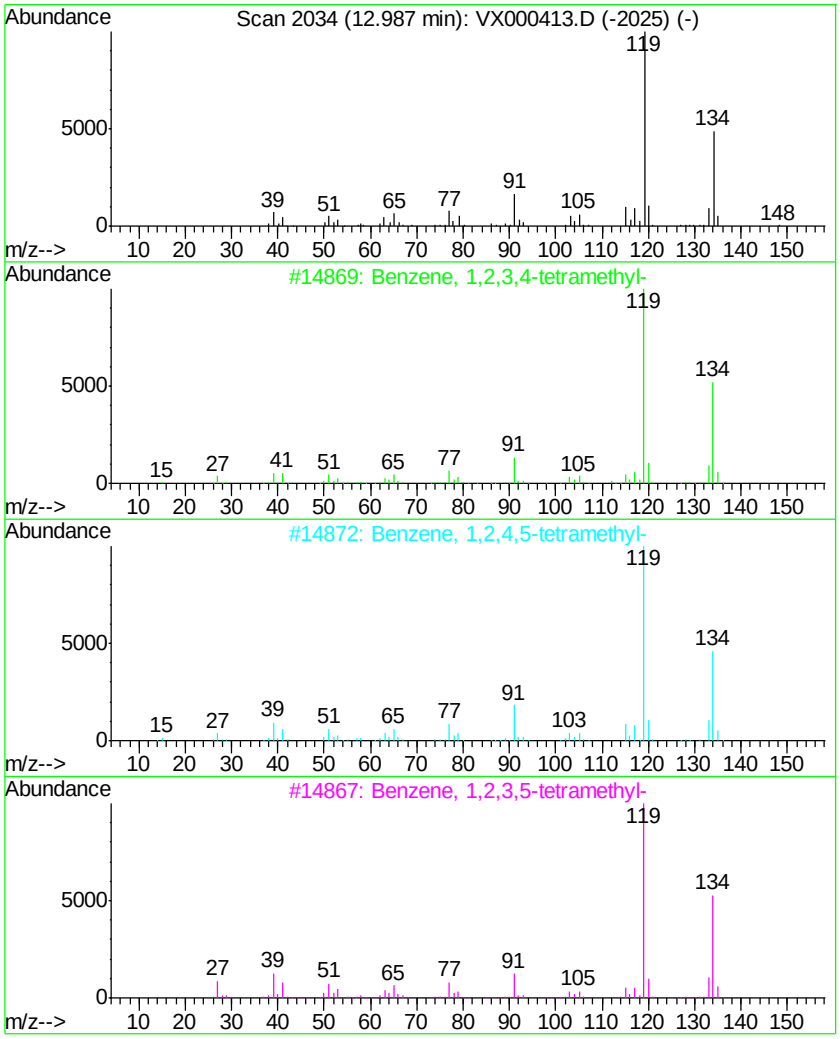
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

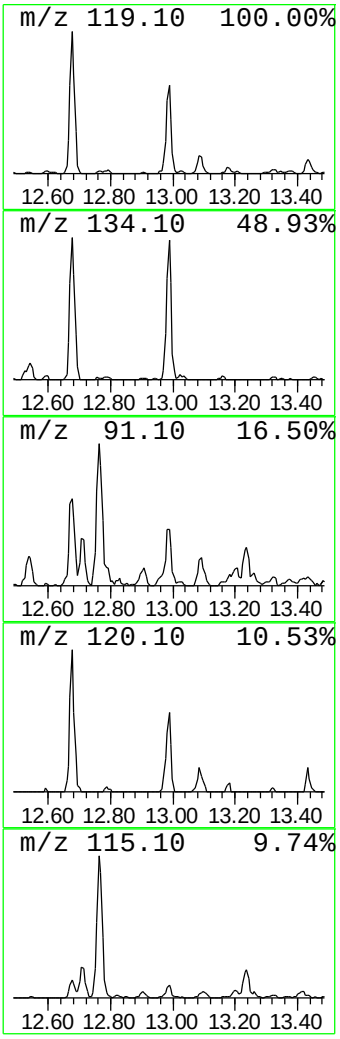
****

Peak Number 10 Benzene, 1,2,3,4-tetramethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.99	7.15 ug/l	65190	1,4-Dichlorobenzene-d4	12.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	97
2	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	97
3	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	95
4	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	94
5	1,3-Cyclopentadiene, 1,2,3,4-tet...	134	C10H14	076089-59-3	94





Tentatively Identified Compound (LSC) summary

Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX032218\
Data File : VX000413.D
Acq On : 22 Mar 2018 18:11
Operator : JC/MD
Sample : J2005-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-7-031918

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

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

TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
Sulfur dioxide	1.28	10.4	ug/l	62745	1	5.67	301814	50.0
Butane, 2-methyl-	1.79	6.5	ug/l	39344	1	5.67	301814	50.0
Di-sec-butyl ether	9.03	13.6	ug/l	136784	3	10.12	504430	50.0
Benzene, 1-etheny...	12.31	41.6	ug/l	379586	4	12.09	456165	50.0
Benzene, 1,4-diet...	12.38	6.3	ug/l	57972	4	12.09	456165	50.0
o-Cymene	12.68	9.8	ug/l	89469	4	12.09	456165	50.0
Benzene, 1-etheny...	12.76	20.4	ug/l	186195	4	12.09	456165	50.0
Benzene, 1,2,3,4-...	12.99	7.2	ug/l	65190	4	12.09	456165	50.0