LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052421\
Data File : VX022159.D
Acq On : 24 May 2021 19:44
Operator : JC/MD
Sample : M2504-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-804

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\82X051921W.M
Title : SW846 8260

Signal : TIC: VX022159.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.270	24	30	43	rBV	645539	1043757	6.87%	0.927%
2	1.374	43	47	53	rBV	2609154	2745581	18.08%	2.440%
3	1.752	103	109	124	rVB	8540823	12385895	81.56%	11.005%
4	1.910	130	135	138	rBV	174124	234824	1.55%	0.209%
5	1.953	138	142	156	rVB	3022244	4347250	28.63%	3.863%
6	2.069	156	161	168	rBV	672481	913997	6.02%	0.812%
7	2.166	172	177	181	rVV	307835	440661	2.90%	0.392%
8	2.215	181	185	195	rVB	611906	912969	6.01%	0.811%
9	2.337	195	205	212	rBV	281047	556009	3.66%	0.494%
10	2.721	259	268	271	rBV4	98519	245069	1.61%	0.218%
11	2.782	271	278	281	rBV	795934	1588584	10.46%	1.412%
12	2.825	281	285	290	rVB	1090608	1964625	12.94%	1.746%
13	3.105	319	331	348	rBV	1221825	2705882	17.82%	2.404%
14	3.324	357	367	378	rBV2	177410	460190	3.03%	0.409%
15	3.452	378	388	400	rBV	432672	968444	6.38%	0.860%
16	3.593	401	411	417	rBV2	156529	385308	2.54%	0.342%
17	3.672	417	424	429	rVV2	231026	534207	3.52%	0.475%
18	3.733	429	434	443	rVB	280389	656670	4.32%	0.583%
19	3.843	443	452	458	rBV	242419	614551	4.05%	0.546%
20	3.952	466	470	485	rVB2	145508	439574	2.89%	0.391%
21	4.111	486	496	505	rVV	232674	606999	4.00%	0.539%
22	4.221	505	514	520	rVV	141604	413696	2.72%	0.368%
23	4.312	520	529	540	rVV	949101	2717574	17.89%	2.415%
24	4.434	540	549	567	rVB3	84446	276920	1.82%	0.246%
25	5.202	666	675	688	rVB2	126646	423203	2.79%	0.376%
26	5.397	691	707	713	rBV4	74900	268678	1.77%	0.239%
27	5.501	713	724	731	rBV5	143055	599716	3.95%	0.533%
28	5.629	738	745	766	rVB	303968	1088191	7.17%	0.967%
29	5.836	766	779	791	rBV	164356	488512	3.22%	0.434%
30	5.964	791	800	808	rBV	61846	158993	1.05%	0.141%
31	6.171	819	834	837	rBV3	122388	380526	2.51%	0.338%
32	6.257	839	848	859	rVV	711019	2266974	14.93%	2.014%
33	6.367	859	866	876	rVB2	99608	283104	1.86%	0.252%
34	6.617	893	907	913	rBV3	64569	167785	1.10%	0.149%
35	6.769	925	932	937	rBV	144983	358264	2.36%	0.318%
36	6.854	938	946	954	rVB3	173872	552349	3.64%	0.491%

LSC Area Percent Report

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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-804

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\82X051921W.M
Title : SW846 8260

37	7.177	988	999	1010	rVB3	113291	277175	1.83%	0.246%
38	7.385	1018	1033	1044	rBV4	287930	836868	5.51%	0.744%
39	7.665	1073	1079	1090	rVB	81494	167448	1.10%	0.149%
40	7.885	1104	1115	1123	rBV3	78000	253386	1.67%	0.225%
41	7.988	1123	1132	1144	rVB	302354	634756	4.18%	0.564%
42	8.110	1144	1152	1156	rBV	301941	640343	4.22%	0.569%
43	8.147	1156	1158	1163	rVV	197372	294561	1.94%	0.262%
44	8.506	1211	1217	1225	rVB2	193949	331687	2.18%	0.295%
45	8.653	1237	1241	1247	rVB	314445	490615	3.23%	0.436%
46	8.726	1247	1253	1259	rBV	240693	384206	2.53%	0.341%
47	8.842	1264	1272	1278	rVB2	92727	196440	1.29%	0.175%
48	9.281	1340	1344	1350	rVB	120349	181096	1.19%	0.161%
49	10.055	1467	1471	1476	rVB	282793	383246	2.52%	0.341%
50	10.201	1489	1495	1501	rBV	3764408	4997834	32.91%	4.441%
51	10.311	1506	1513	1528	rVB	10604096	15186633	100.00%	13.494%
52	10.646	1562	1568	1578	rVB	1318616	1689836	11.13%	1.501%
53	10.963	1613	1620	1628	rBV	443193	581443	3.83%	0.517%
54	11.085	1635	1640	1645	rBV	244889	301528	1.99%	0.268%
55	11.305	1667	1676	1683	rBV	931546	1207425	7.95%	1.073%
56	11.384	1684	1689	1696	rVV	3585696	6373469	41.97%	5.663%
57	11.457	1696	1701	1707	rVB	2715711	3266406	21.51%	2.902%
58	11.616	1722	1727	1736	rVB	2145336	2591065	17.06%	2.302%
59	11.756	1745	1750	1755	rVB	7434383	9547854	62.87%	8.484%
60	12.024	1789	1794	1800	rVB	329754	424635	2.80%	0.377%
61	12.091	1800	1805	1810	rBV	1766026	2095220	13.80%	1.862%
62	12.250	1825	1831	1838	rBV2	1484368	2275998	14.99%	2.022%
63	12.323	1838	1843	1850	rVB2	669835	951845	6.27%	0.846%
64	12.463	1862	1866	1872	rVB	146265	186903	1.23%	0.166%
65	12.536	1872	1878	1880	rBV	425682	566929	3.73%	0.504%
66	12.561	1880	1882	1886	rVB	330345	323989	2.13%	0.288%
67	12.615	1886	1891	1894	rBV	898133	1038341	6.84%	0.923%
68	12.646	1894	1896	1901	rVB	161790	186489	1.23%	0.166%
69	12.701	1901	1905	1913	rBV2	786108	1086353	7.15%	0.965%
70	12.853	1925	1930	1935	rVB2	177936	230230	1.52%	0.205%
71	12.926	1935	1942	1945	rBV	537500	654493	4.31%	0.582%
72	12.969	1945	1949	1954	rVB	553632	684303	4.51%	0.608%
73	13.170	1978	1982	1987	rVB	472434	552296	3.64%	0.491%
74	13.292	1998	2002	2008	rVB2	1155528	1566193	10.31%	1.392%
75	13.426	2020	2024	2032	rVB	136719	172198	1.13%	0.153%
76	13.548	2040	2044	2047	rBV	150647	196888	1.30%	0.175%

LSC Area Percent Report

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Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-804

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

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Title : SW846 8260

77	13.585	2047	2050	2056	rVB3	102833	168893	1.11%	0.150%
78	13.670	2061	2064	2069	rVB2	148921	223587	1.47%	0.199%
79	13.780	2075	2082	2088	rBV	1390766	1720153	11.33%	1.528%
80	14.639	2218	2223	2229	rVB	697329	849620	5.59%	0.755%
81	14.780	2241	2246	2259	rVB	287211	379278	2.50%	0.337%

Sum of corrected areas: 112545685

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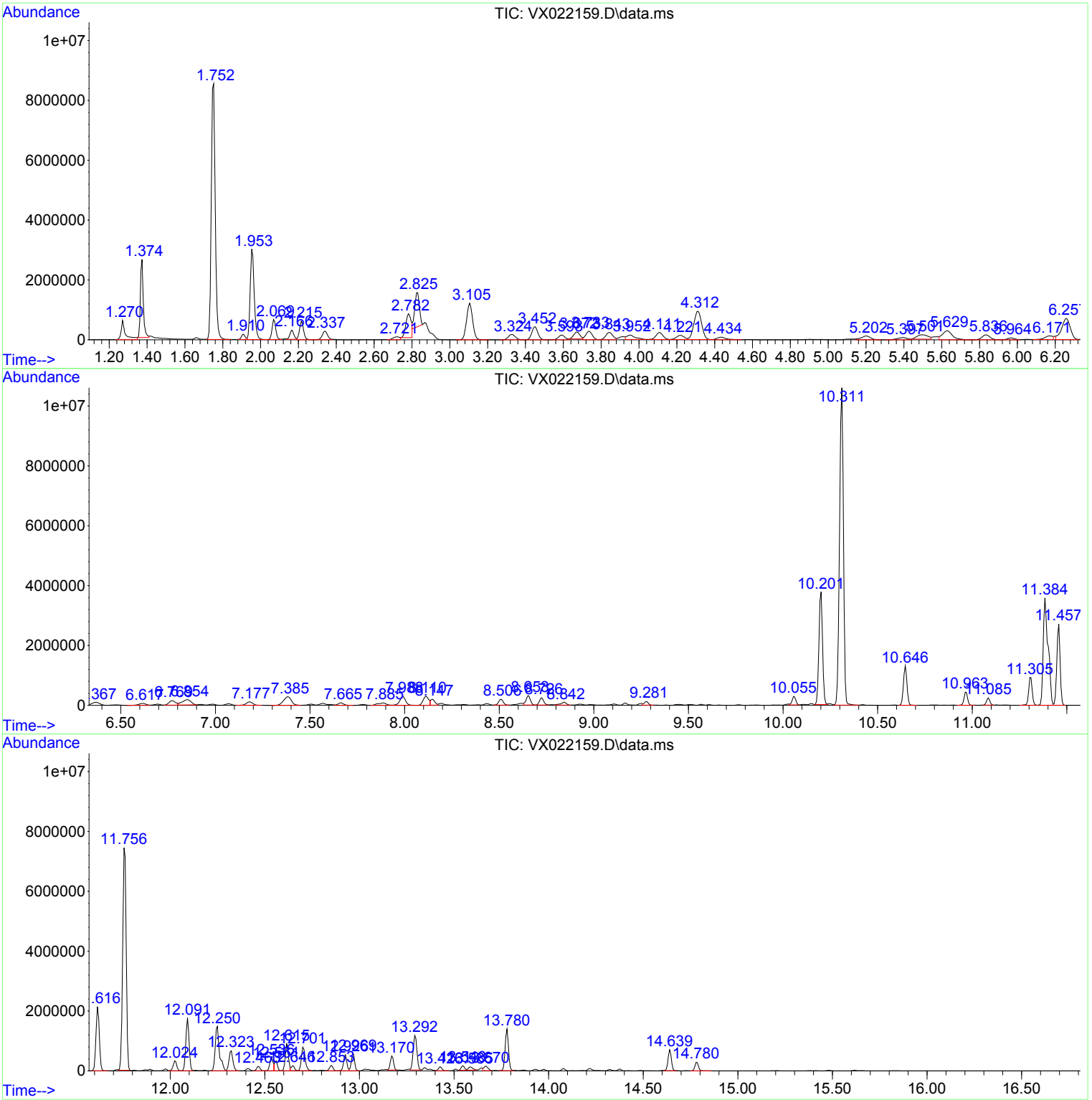
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-804

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052421\
Data File : VX022159.D
Acq On : 24 May 2021 19:44
Operator : JC/MD
Sample : M2504-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-804

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

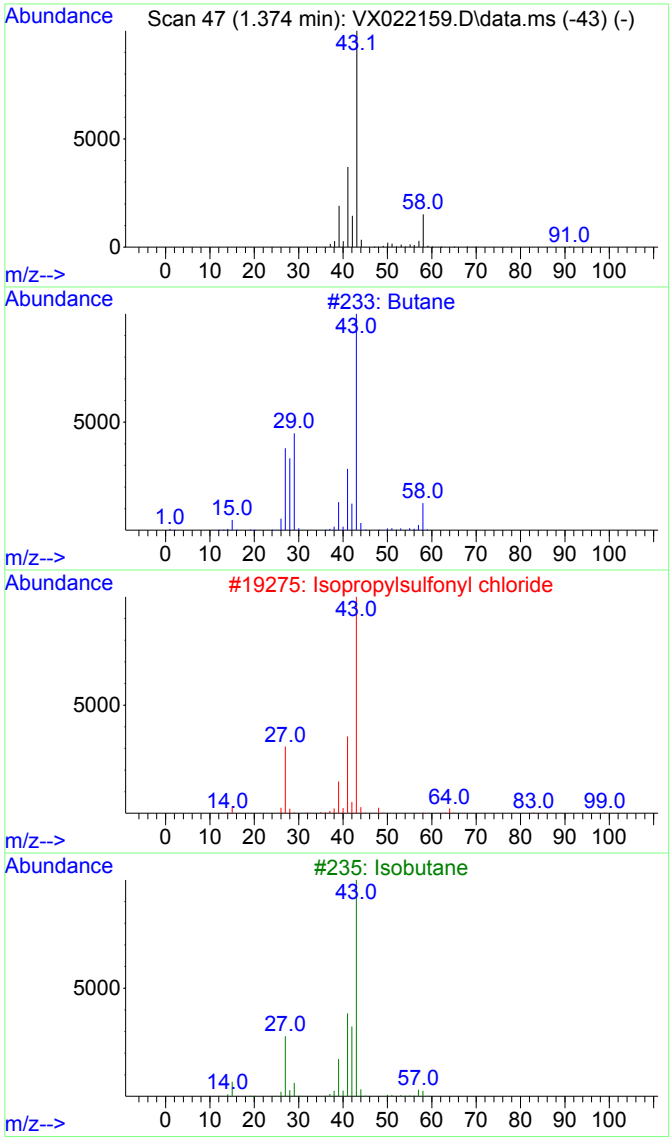
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

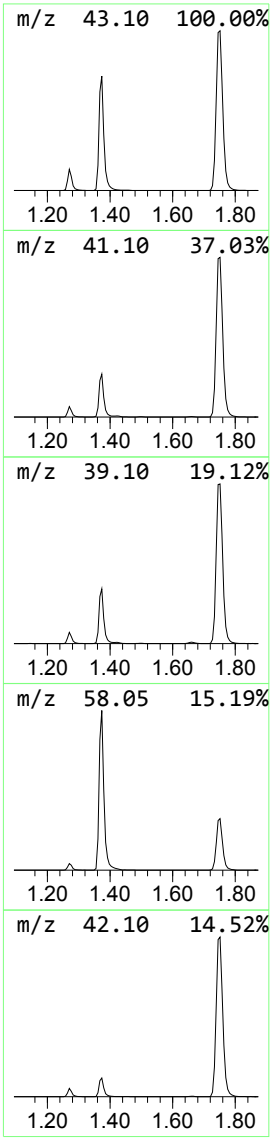
****

Peak Number 1 Butane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.374	228.91 ug/l	2745580	Pentafluorobenzene	5.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane	58	C4H10	000106-97-8	80
2	Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9
3	Isobutane	58	C4H10	000075-28-5	9
4	Propane, 1-nitro-	89	C3H7NO2	000108-03-2	9
5	Diazene, dimethyl-	58	C2H6N2	000503-28-6	5





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Operator : JC/MD
Sample : M2504-06
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ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-804

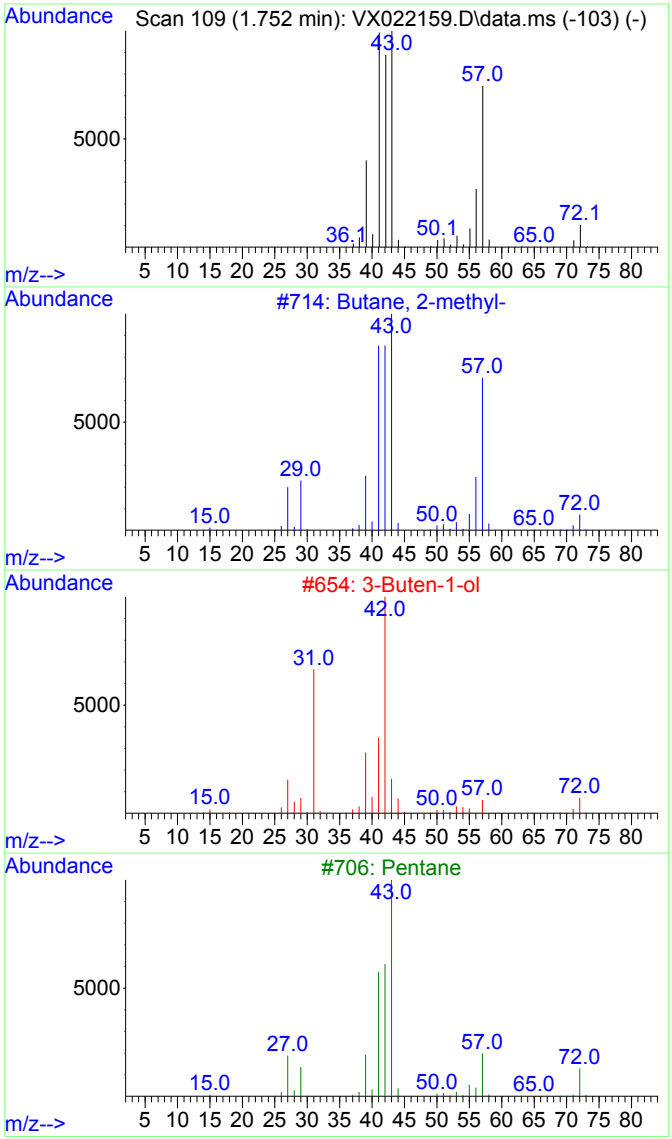
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

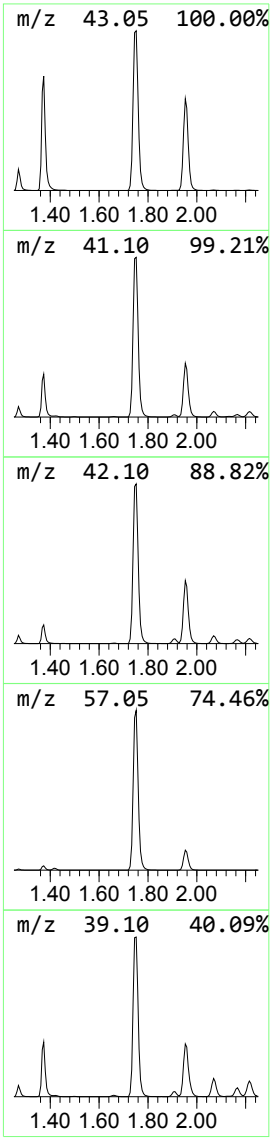
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Butane, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.752	1032.65 ug/l	12385900	Pentafluorobenzene	5.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	87
2	3-Buten-1-ol	72	C4H8O	000627-27-0	38
3	Pentane	72	C5H12	000109-66-0	36
4	Oxirane, trimethyl-	86	C5H10O	005076-19-7	25
5	1-Propene, 2-methyl-	56	C4H8	000115-11-7	22





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Data File : VX022159.D
Acq On : 24 May 2021 19:44
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Sample : M2504-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-804

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
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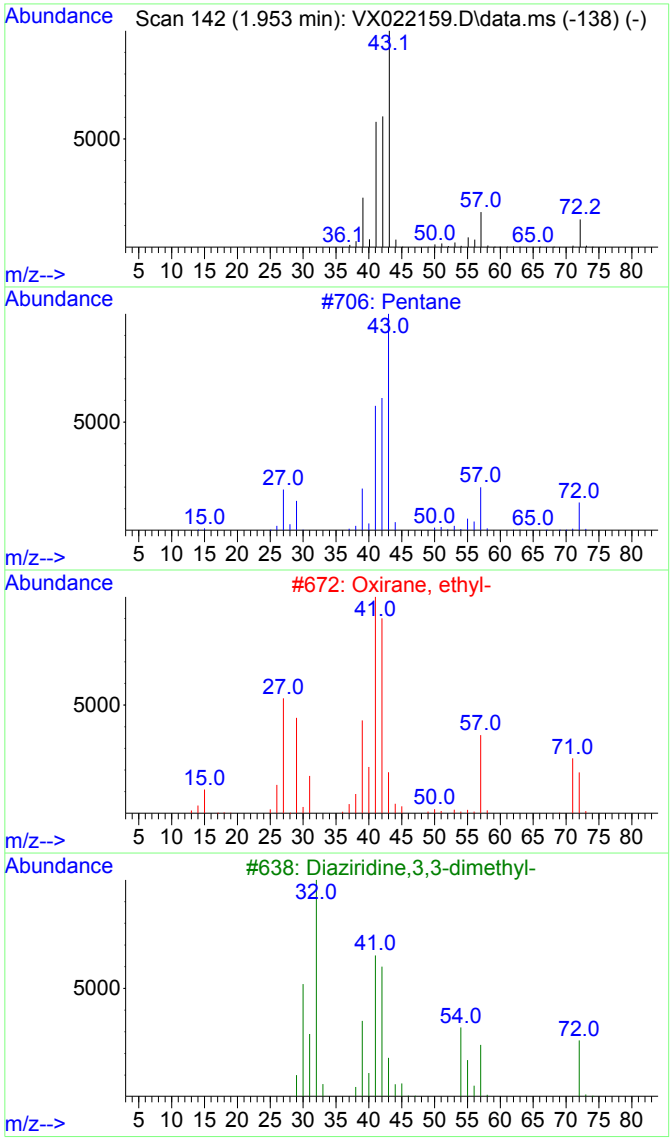
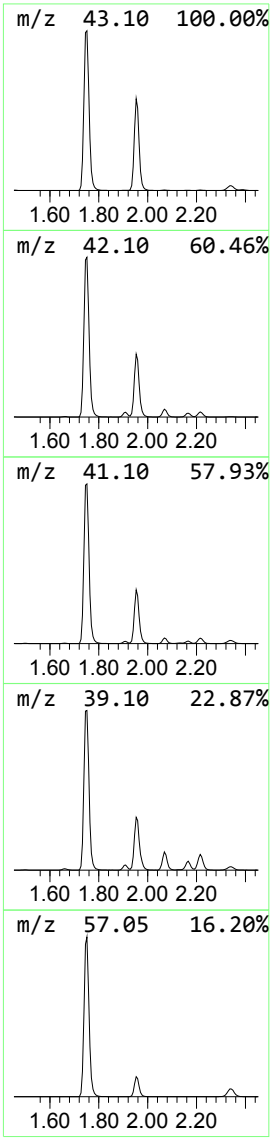
****
Peak Number 3 Pentane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.953	362.44 ug/l	4347250	Pentafluorobenzene	5.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane	72	C5H12	000109-66-0	91
2	Oxirane, ethyl-	72	C4H8O	000106-88-7	47
3	Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	38
4	Butane, 2-methyl-	72	C5H12	000078-78-4	38
5	Butanenitrile, 3-methyl-	83	C5H9N	000625-28-5	9





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ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-804

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
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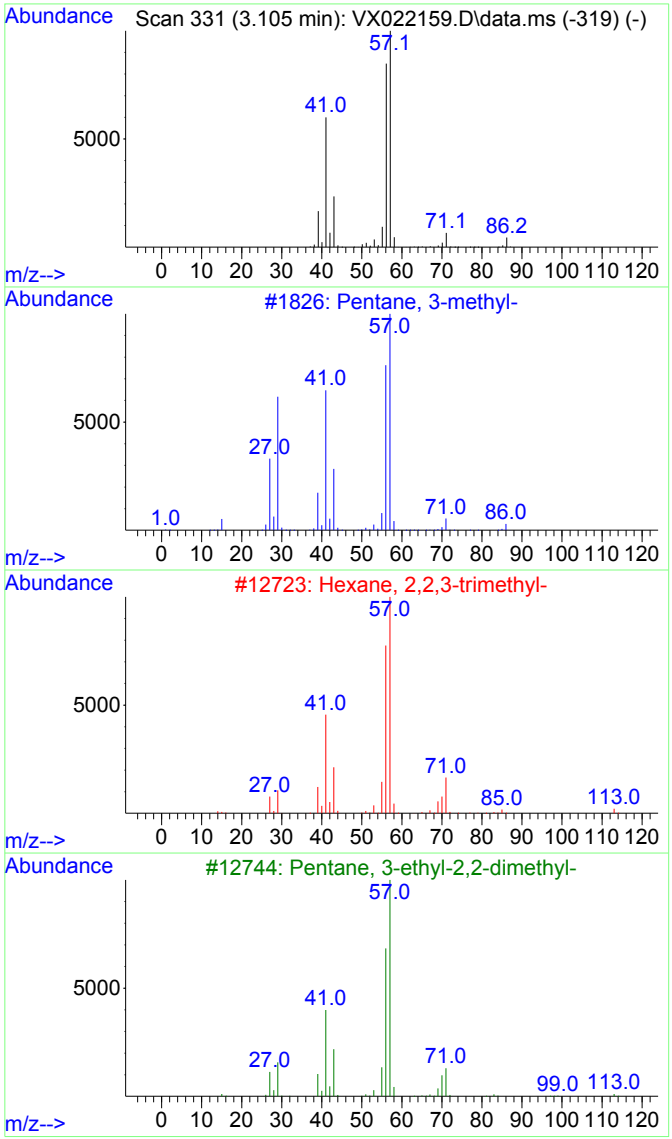
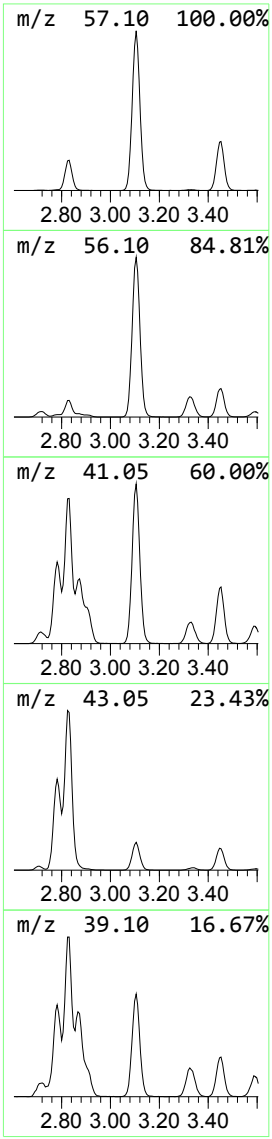
****
Peak Number 4 Pentane, 3-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.105	225.60 ug/l	2705880	Pentafluorobenzene	5.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 3-methyl-	86	C6H14	000096-14-0	91
2	Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	83
3	Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	43
4	3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	42
5	Sulphuric acid dibutyl ester	210	C8H18O4S	000625-22-9	40





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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-804

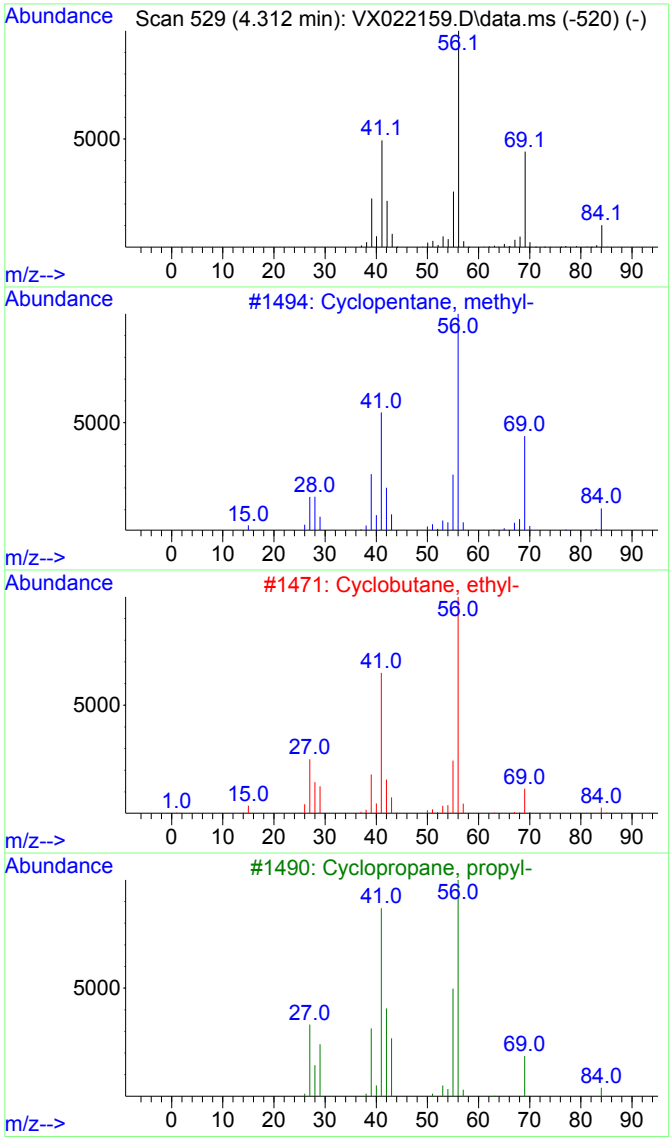
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

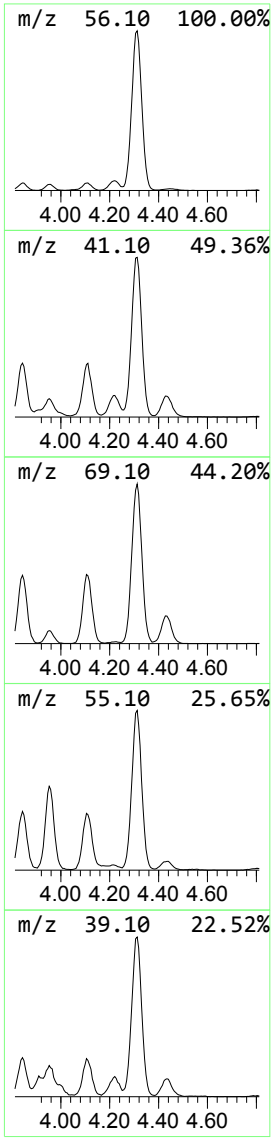
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Cyclopentane, methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.312	226.57 ug/l	2717570	Pentafluorobenzene	5.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2	Cyclobutane, ethyl-	84	C6H12	004806-61-5	72
3	Cyclopropane, propyl-	84	C6H12	002415-72-7	56
4	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	50
5	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	50





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Data File : VX022159.D
Acq On : 24 May 2021 19:44
Operator : JC/MD
Sample : M2504-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-804

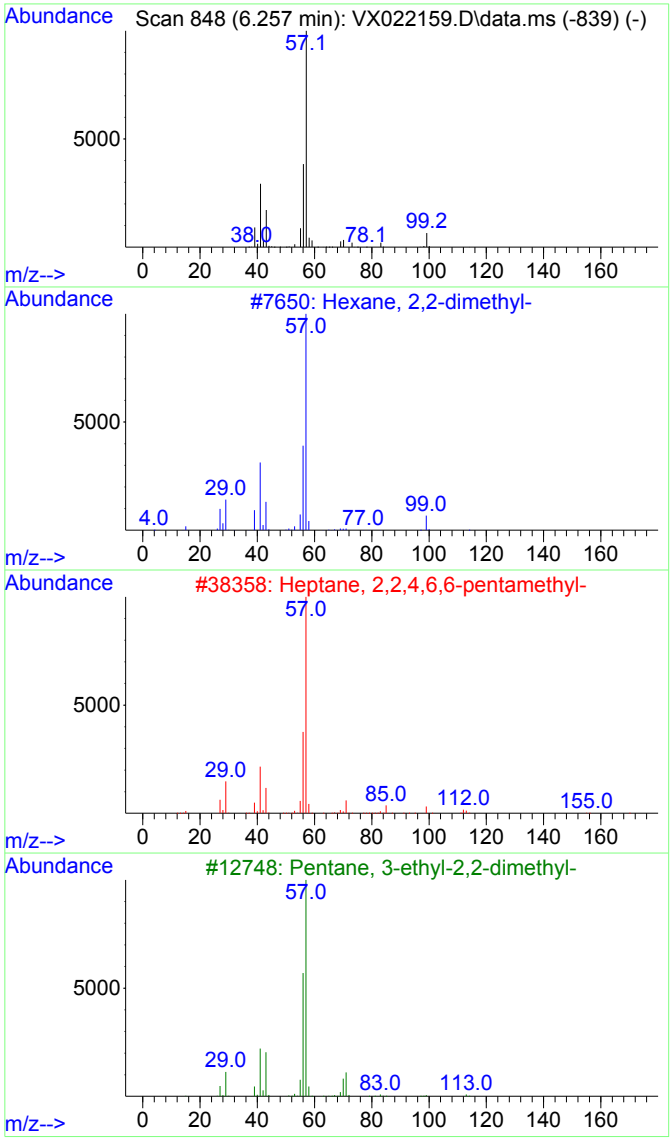
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

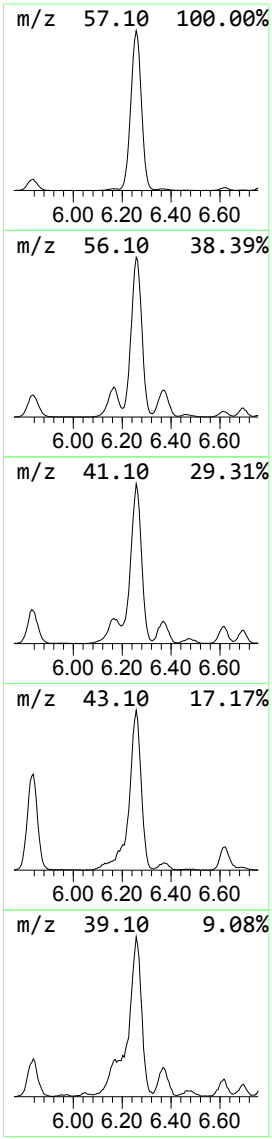
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Hexane, 2,2-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.257	316.38 ug/l	2266970	1,4-Difluorobenzene	6.769

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	72
2	Heptane, 2,2,4,6,6-pentamethyl-	170	C12H26	013475-82-6	72
3	Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	64
4	Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	64
5	Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052421\
Data File : VX022159.D
Acq On : 24 May 2021 19:44
Operator : JC/MD
Sample : M2504-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-804

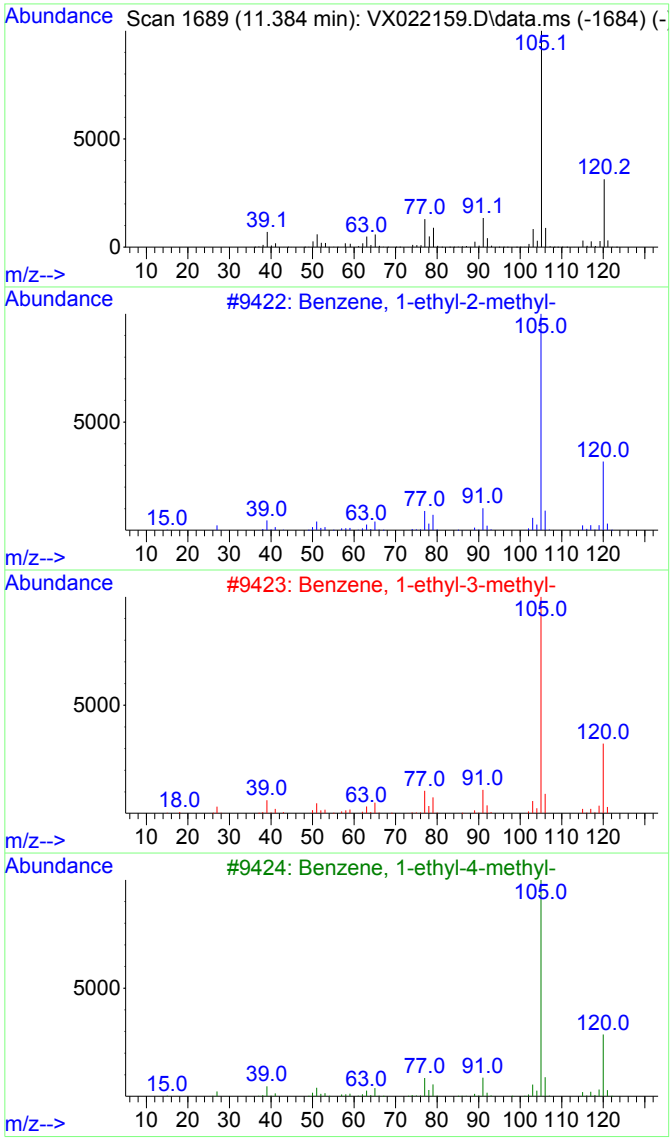
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

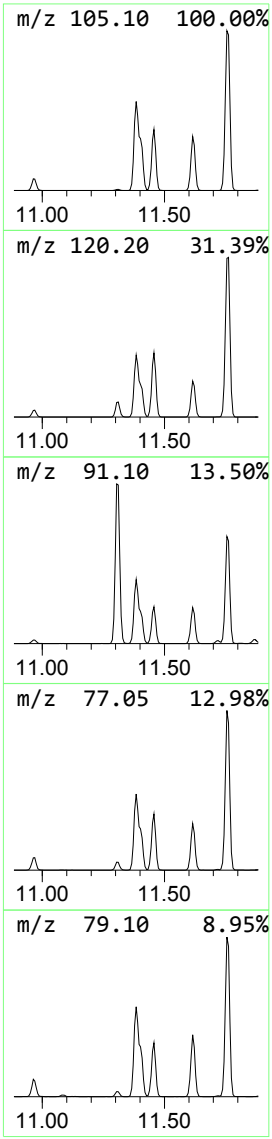
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, 1-ethyl-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.384	750.46 ug/l	6373470	1,4-Dichlorobenzene-d4	12.030

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	94
3	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4	Mesitylene	120	C9H12	000108-67-8	91
5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	90





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052421\
Data File : VX022159.D
Acq On : 24 May 2021 19:44
Operator : JC/MD
Sample : M2504-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-804

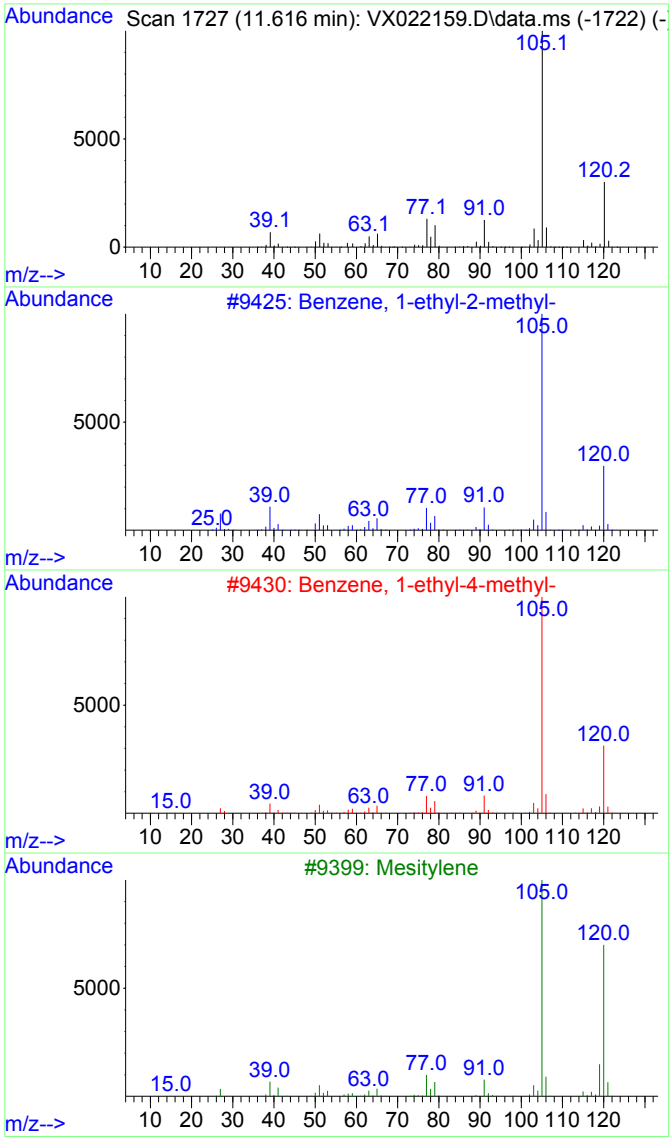
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

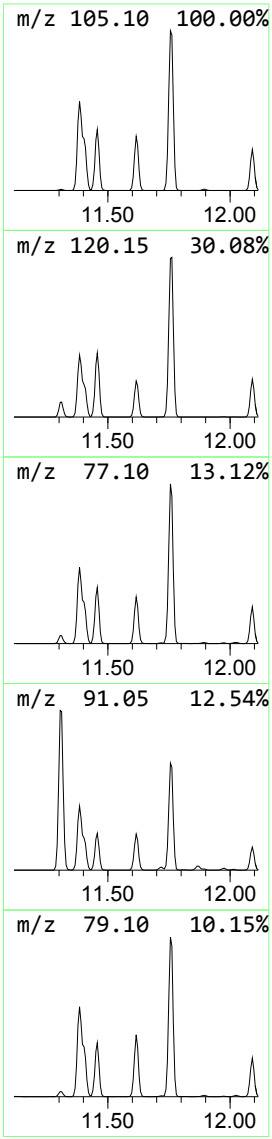
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, 1-ethyl-4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.616	305.09 ug/l	2591070	1,4-Dichlorobenzene-d4	12.030

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
3	Mesitylene	120	C9H12	000108-67-8	91
4	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052421\
Data File : VX022159.D
Acq On : 24 May 2021 19:44
Operator : JC/MD
Sample : M2504-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-804

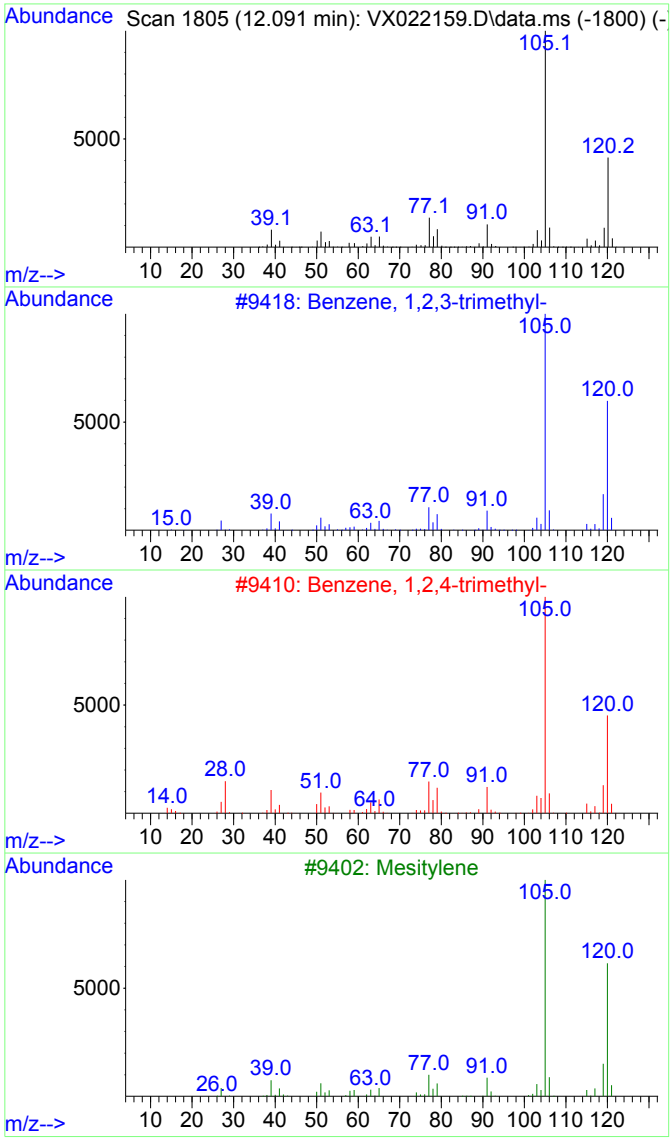
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

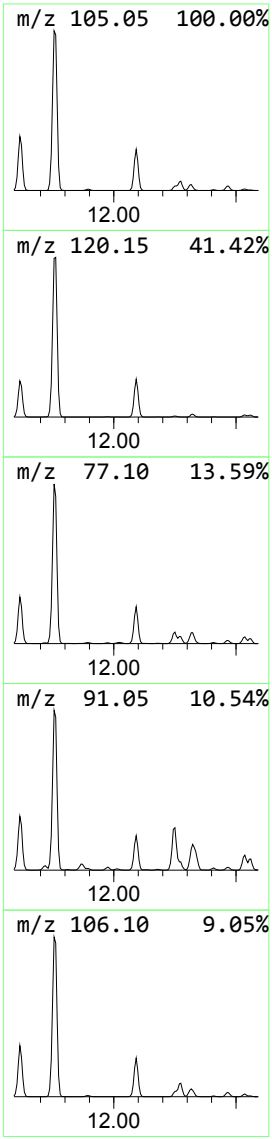
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, 1,2,3-trimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.091	246.71 ug/l	2095220	1,4-Dichlorobenzene-d4	12.030

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
2	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	94
3	Mesitylene	120	C9H12	000108-67-8	91
4	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052421\
Data File : VX022159.D
Acq On : 24 May 2021 19:44
Operator : JC/MD
Sample : M2504-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-804

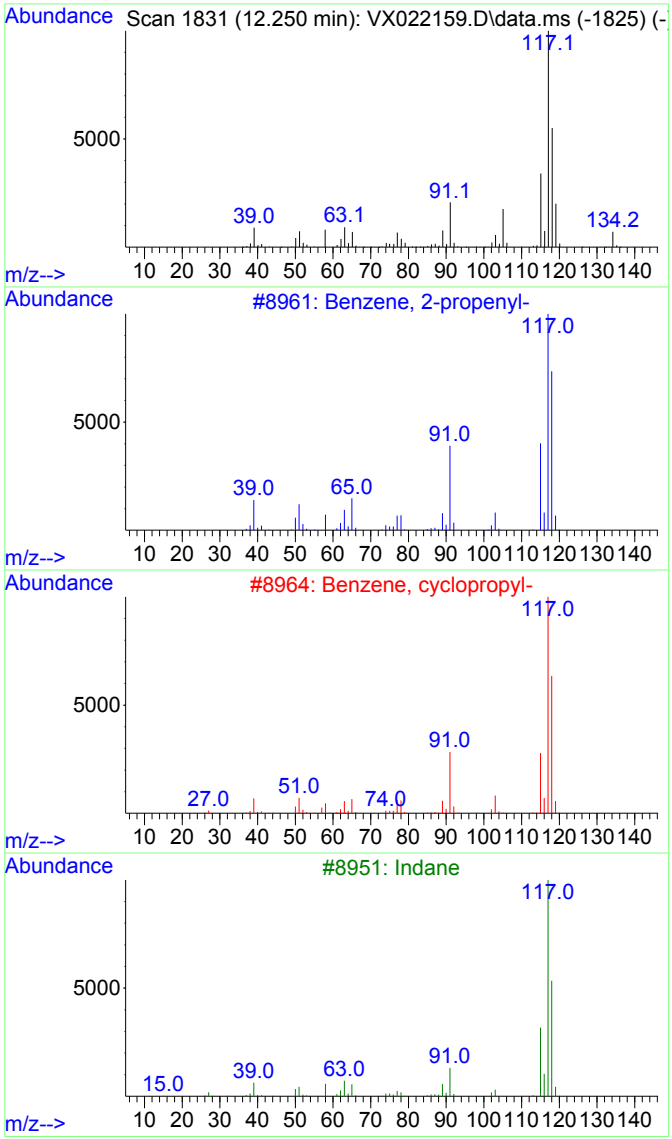
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

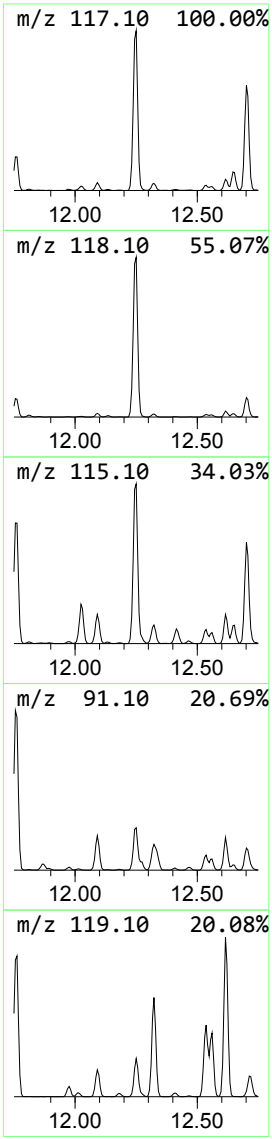
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Benzene, 2-propenyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.250	268.00 ug/l	2276000	1,4-Dichlorobenzene-d4	12.030

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-propenyl-	118	C9H10	000300-57-2	76
2	Benzene, cyclopropyl-	118	C9H10	000873-49-4	70
3	Indane	118	C9H10	000496-11-7	70
4	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	50
5	Benzene, 1-propenyl-	118	C9H10	000637-50-3	49





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052421\
Data File : VX022159.D
Acq On : 24 May 2021 19:44
Operator : JC/MD
Sample : M2504-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-804

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.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
Butane	1.374	228.9	ug/l	2745580	1	5.562	599716	50.0
Butane, 2-methyl-	1.752	1032.7	ug/l	12385900	1	5.562	599716	50.0
Pentane	1.953	362.4	ug/l	4347250	1	5.562	599716	50.0
Pentane, 3-methyl-	3.105	225.6	ug/l	2705880	1	5.562	599716	50.0
Cyclopentane, m...	4.312	226.6	ug/l	2717570	1	5.562	599716	50.0
Hexane, 2,2-dim...	6.257	316.4	ug/l	2266970	2	6.769	358264	50.0
Benzene, 1-ethy...	11.384	750.5	ug/l	6373470	4	12.030	424635	50.0
Benzene, 1-ethy...	11.616	305.1	ug/l	2591070	4	12.030	424635	50.0
Benzene, 1,2,3-...	12.091	246.7	ug/l	2095220	4	12.030	424635	50.0
Benzene, 2-prop...	12.250	268.0	ug/l	2276000	4	12.030	424635	50.0