LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052022\
Data File : VX028858.D
Acq On : 20 May 2022 18:06
Operator : JC/MD
Sample : N2943-16
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-22

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\82X051222W.M
Title : SW846 8260

Signal : TIC: VX028858.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.264	19	29	42	rBV2	97564	210611	15.44%	1.244%
2	1.368	43	46	52	rVB	43215	51145	3.75%	0.302%
3	1.752	104	109	121	rVB	259478	358805	26.31%	2.119%
4	1.953	137	142	149	rVB	75667	108229	7.94%	0.639%
5	2.215	180	185	193	rVB	24504	38365	2.81%	0.227%
6	2.343	199	206	210	rBV	15014	30006	2.20%	0.177%
7	2.538	228	238	246	rBV	8197	18300	1.34%	0.108%
8	2.782	259	278	282	rBV2	54298	129597	9.50%	0.765%
9	2.825	282	285	288	rVV2	51622	93668	6.87%	0.553%
10	2.867	288	292	301	rVV	64485	140722	10.32%	0.831%
11	2.959	301	307	322	rVV2	36045	87068	6.38%	0.514%
12	3.111	322	332	347	rVB3	98758	247620	18.16%	1.462%
13	3.745	426	436	445	rBV4	10324	37333	2.74%	0.220%
14	3.843	445	452	457	rVV2	10181	24753	1.82%	0.146%
15	4.221	505	514	518	rVV4	6218	17537	1.29%	0.104%
16	4.306	518	528	540	rVV	166141	476305	34.93%	2.813%
17	4.428	542	548	562	rVB6	9203	29967	2.20%	0.177%
18	5.202	668	675	684	rVB6	6595	21489	1.58%	0.127%
19	5.391	694	706	713	rBV2	160067	468316	34.34%	2.766%
20	5.477	713	720	726	rVV2	118460	346868	25.43%	2.049%
21	5.556	726	733	743	rVB	244261	664436	48.72%	3.924%
22	5.842	769	780	789	rBV5	11430	36445	2.67%	0.215%
23	5.958	789	799	806	rBV	170214	449015	32.92%	2.652%
24	6.044	806	813	825	rVB	206757	547783	40.17%	3.235%
25	6.251	843	847	856	rVB3	24279	66225	4.86%	0.391%
26	6.361	856	865	876	rVB4	20703	64944	4.76%	0.384%
27	6.763	921	931	941	rBV	414568	1004300	73.64%	5.931%
28	7.178	991	999	1007	rVB3	12879	29457	2.16%	0.174%
29	7.379	1020	1032	1046	rBV4	67691	189294	13.88%	1.118%
30	7.659	1073	1078	1085	rVB2	7879	14725	1.08%	0.087%
31	7.775	1090	1097	1104	rBV3	8068	16557	1.21%	0.098%
32	7.860	1104	1111	1112	rBV2	16166	27596	2.02%	0.163%
33	7.879	1112	1114	1123	rVV4	18796	37164	2.73%	0.219%
34	7.988	1123	1132	1141	rVB2	17122	40882	3.00%	0.241%
35	8.110	1143	1152	1155	rBV	35731	75346	5.52%	0.445%
36	8.147	1155	1158	1164	rVV	40691	66050	4.84%	0.390%

LSC Area Percent Report

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Operator : JC/MD
Sample : N2943-16
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-22

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\82X051222W.M
Title : SW846 8260

37	8.427	1199	1204	1210	rVB2	11111	17168	1.26%	0.101%
38	8.507	1210	1217	1225	rVB	36968	66983	4.91%	0.396%
39	8.653	1225	1241	1249	rBV	857876	1363793	100.00%	8.054%
40	8.842	1266	1272	1281	rVV7	7010	15642	1.15%	0.092%
41	8.958	1287	1291	1300	rVB4	31082	58247	4.27%	0.344%
42	9.049	1300	1306	1312	rBV	28307	47667	3.50%	0.282%
43	9.165	1320	1325	1335	rBV	28634	47985	3.52%	0.283%
44	9.458	1365	1373	1377	rBV5	16112	38807	2.85%	0.229%
45	9.500	1377	1380	1387	rVB6	7753	15403	1.13%	0.091%
46	10.055	1465	1471	1477	rBV	854499	1120189	82.14%	6.616%
47	10.195	1489	1494	1500	rBV	193961	242047	17.75%	1.429%
48	10.305	1509	1512	1517	rVB2	20799	28075	2.06%	0.166%
49	10.964	1615	1620	1627	rBV	206320	254317	18.65%	1.502%
50	11.085	1634	1640	1645	rBV	646643	835432	61.26%	4.934%
51	11.305	1671	1676	1685	rVB	260821	317083	23.25%	1.873%
52	11.396	1685	1691	1696	rBV	11746	21846	1.60%	0.129%
53	11.616	1722	1727	1735	rVB	46656	60137	4.41%	0.355%
54	11.713	1738	1743	1746	rVV3	12350	17157	1.26%	0.101%
55	11.756	1746	1750	1756	rVB	26917	35452	2.60%	0.209%
56	11.866	1763	1768	1770	rBV	46959	60396	4.43%	0.357%
57	11.890	1770	1772	1781	rVB	47617	57377	4.21%	0.339%
58	12.024	1788	1794	1799	rVV	1010972	1234986	90.56%	7.294%
59	12.085	1802	1804	1810	rVB	18887	23918	1.75%	0.141%
60	12.177	1815	1819	1824	rBV	20992	26219	1.92%	0.155%
61	12.244	1824	1830	1837	rBV2	871974	1073150	78.69%	6.338%
62	12.317	1837	1842	1852	rVB2	49951	89233	6.54%	0.527%
63	12.408	1852	1857	1861	rBV2	54959	71102	5.21%	0.420%
64	12.463	1861	1866	1872	rVB	133555	158824	11.65%	0.938%
65	12.530	1872	1877	1883	rBV	18668	23797	1.74%	0.141%
66	12.610	1883	1890	1893	rBV2	15126	23652	1.73%	0.140%
67	12.646	1893	1896	1900	rVV	83746	100006	7.33%	0.591%
68	12.701	1900	1905	1912	rVB	415172	510165	37.41%	3.013%
69	12.847	1919	1929	1934	rVB2	47324	71063	5.21%	0.420%
70	12.920	1934	1941	1945	rBV	220154	288267	21.14%	1.702%
71	12.963	1945	1948	1954	rVB	180808	210504	15.44%	1.243%
72	13.030	1954	1959	1965	rVB3	23138	37257	2.73%	0.220%
73	13.140	1974	1977	1979	rVV2	29364	37794	2.77%	0.223%
74	13.170	1979	1982	1991	rVB	89490	127654	9.36%	0.754%
75	13.250	1991	1995	1998	rBV3	18667	26358	1.93%	0.156%
76	13.292	1998	2002	2007	rVV	282920	354849	26.02%	2.096%

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ClientSampleId :
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Integration Parameters: RTEINT.P
Integrator: RTE
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Title : SW846 8260

77	13.347	2007	2011	2013	rVV3	28376	47046	3.45%	0.278%
78	13.372	2013	2015	2018	rVV	19547	24060	1.76%	0.142%
79	13.427	2019	2024	2031	rVB	103942	140002	10.27%	0.827%
80	13.500	2031	2036	2040	rBV2	20889	35224	2.58%	0.208%
81	13.548	2040	2044	2046	rVV	58197	80703	5.92%	0.477%
82	13.579	2046	2049	2056	rVV3	74083	155518	11.40%	0.918%
83	13.646	2056	2060	2061	rVV	45038	68190	5.00%	0.403%
84	13.664	2061	2063	2070	rVB2	68595	94302	6.91%	0.557%
85	13.774	2073	2081	2090	rBV	179414	255756	18.75%	1.510%
86	13.859	2090	2095	2100	rBV3	26919	48794	3.58%	0.288%
87	13.926	2100	2106	2110	rBV2	41853	56875	4.17%	0.336%
88	13.975	2110	2114	2117	rVB	19176	23442	1.72%	0.138%
89	14.073	2126	2130	2138	rBV	31261	44436	3.26%	0.262%
90	14.213	2149	2153	2160	rBV	41478	69137	5.07%	0.408%
91	14.323	2167	2171	2175	rBV	25404	32580	2.39%	0.192%
92	14.371	2175	2179	2184	rVB	32023	41280	3.03%	0.244%
93	14.481	2192	2197	2202	rBV2	25355	36414	2.67%	0.215%
94	14.603	2210	2217	2221	rBV4	12609	25360	1.86%	0.150%
95	14.780	2241	2246	2256	rBV	121869	161415	11.84%	0.953%
96	15.615	2377	2383	2392	rBV3	9167	14923	1.09%	0.088%

Sum of corrected areas: 16932381

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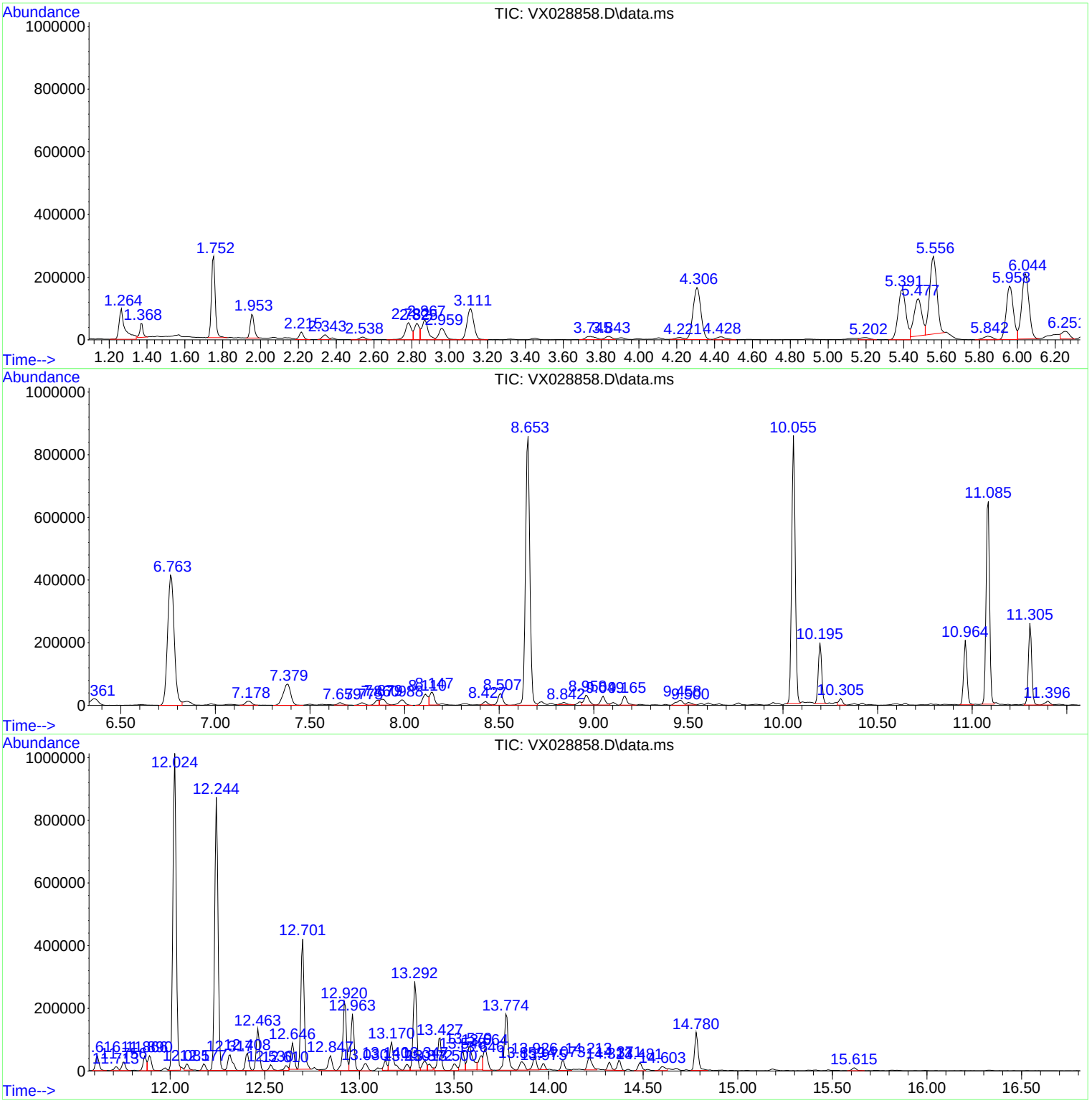
Instrument :
MSVOA_X
ClientSampleId :
MW-22

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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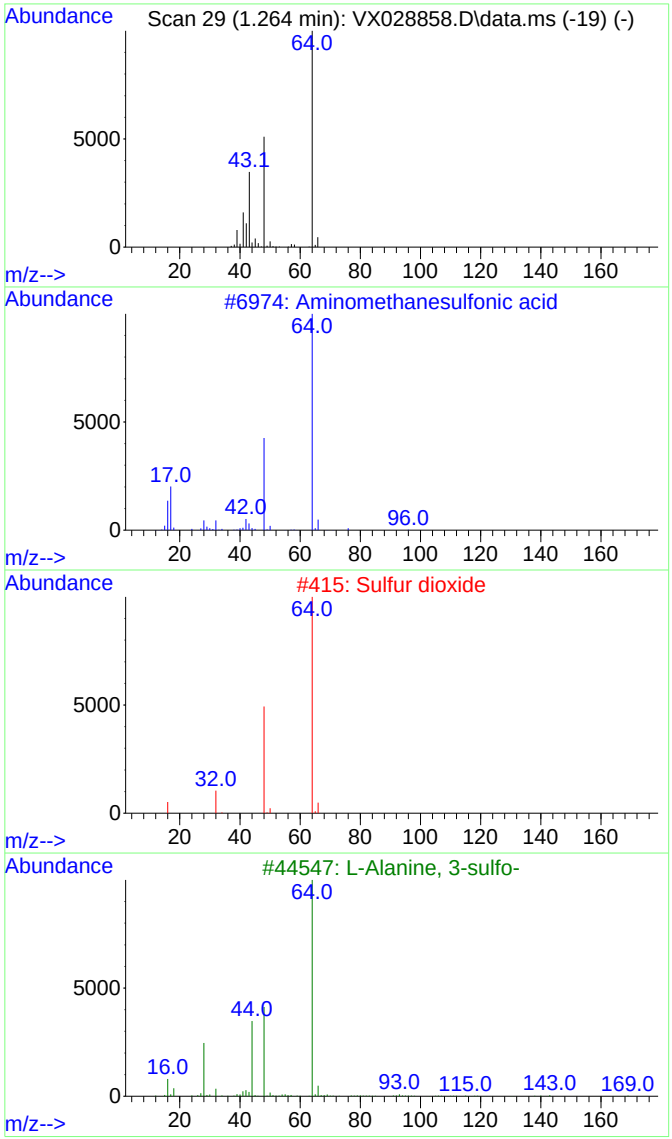
Quant Title : SW846 8260

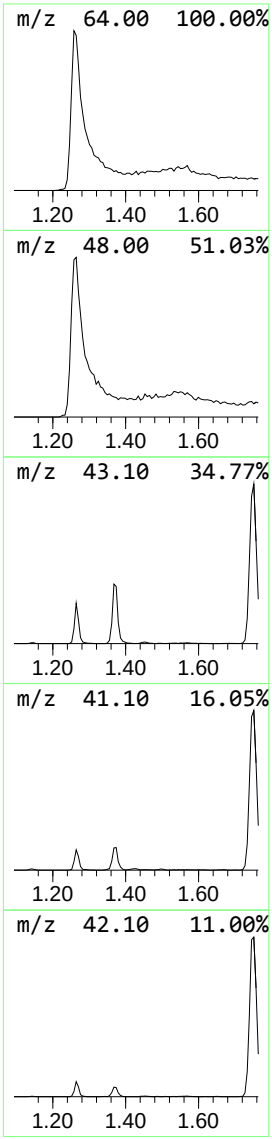
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Aminomethanesulfonic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.264	15.85 ug/l	210611	Pentafluorobenzene	5.556

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





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ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-22

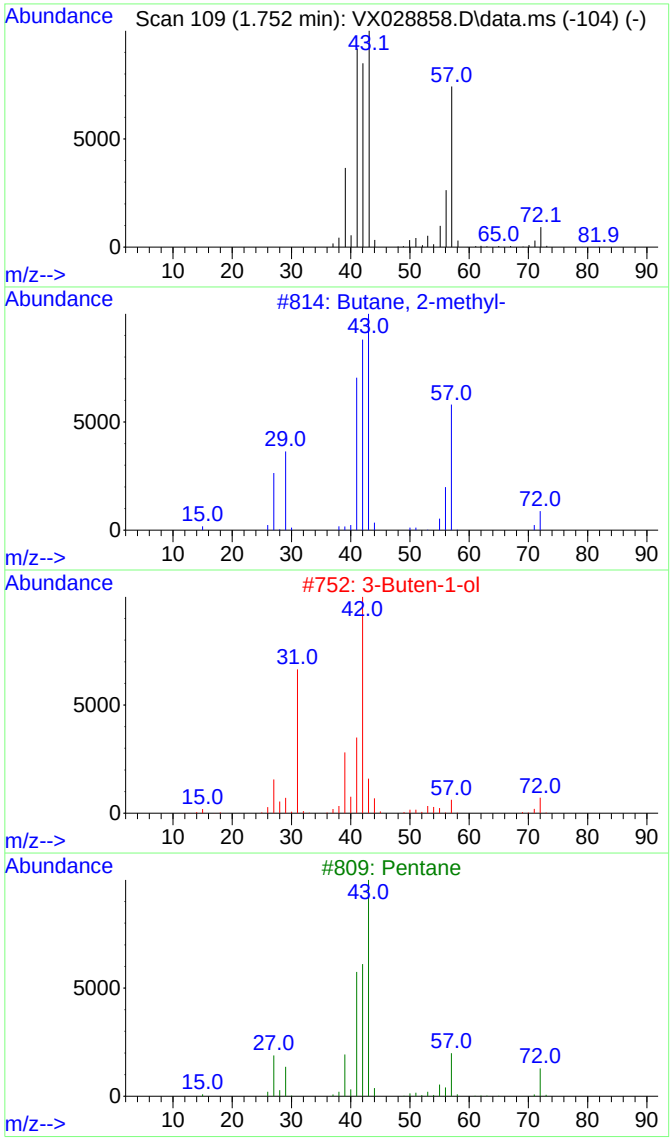
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

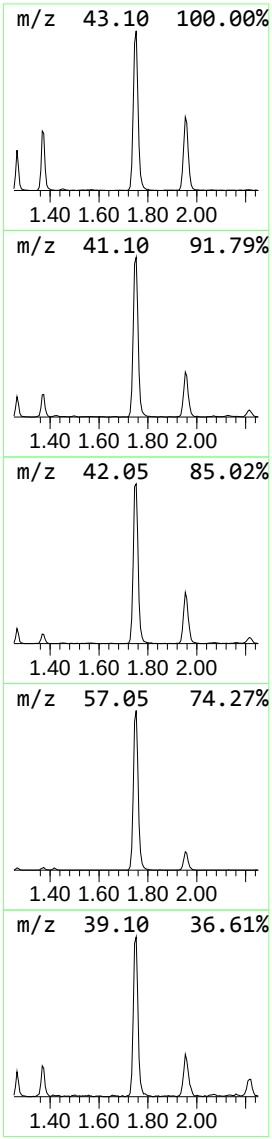
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.752	27.00 ug/l	358805	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	86
2	3-Buten-1-ol	72	C4H8O	000627-27-0	43
3	Pentane	72	C5H12	000109-66-0	28
4	Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	12
5	1-Butene	56	C4H8	000106-98-9	10





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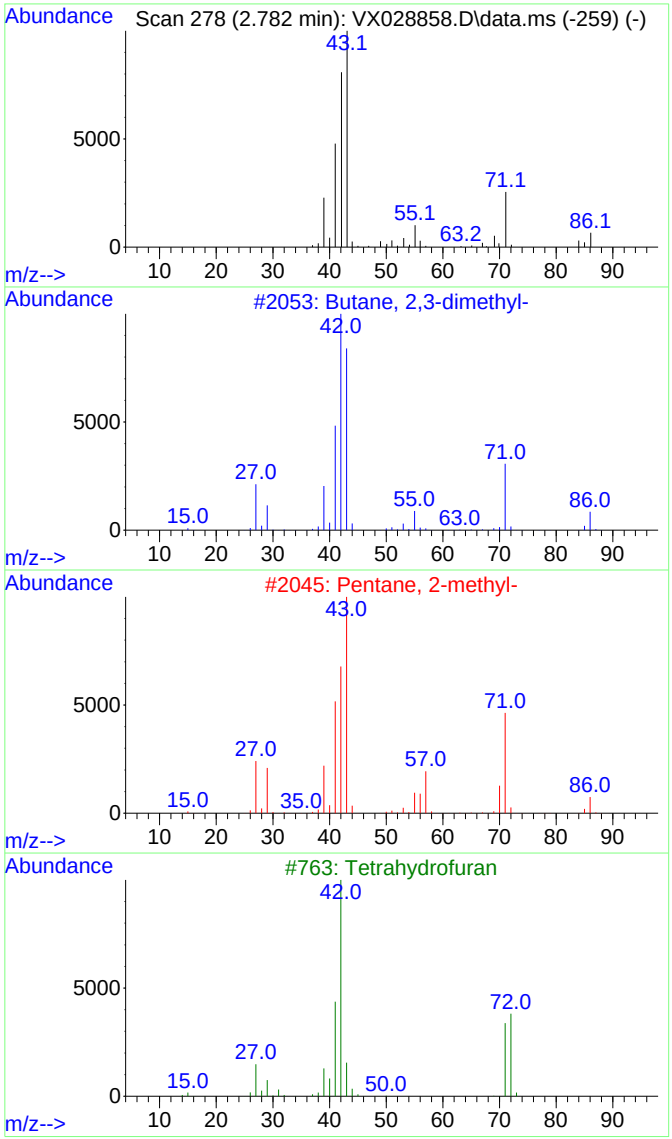
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

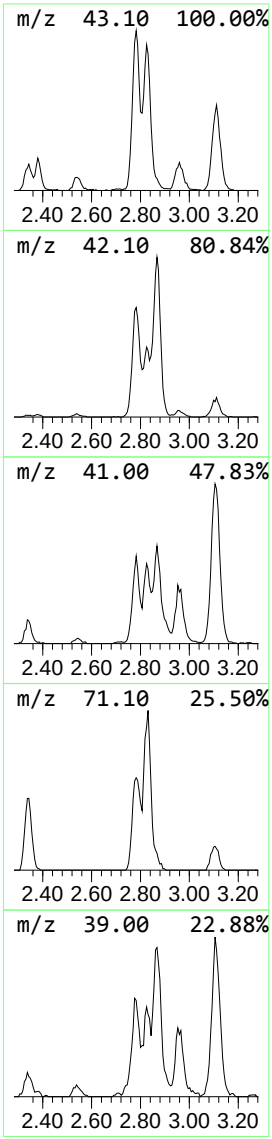
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Butane, 2,3-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.782	9.75 ug/l	129597	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	80
2	Pentane, 2-methyl-	86	C6H14	000107-83-5	45
3	Tetrahydrofuran	72	C4H8O	000109-99-9	36
4	1-Pentene	70	C5H10	000109-67-1	28
5	Propanoyl chloride, 2-methyl-	106	C4H7ClO	000079-30-1	10





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ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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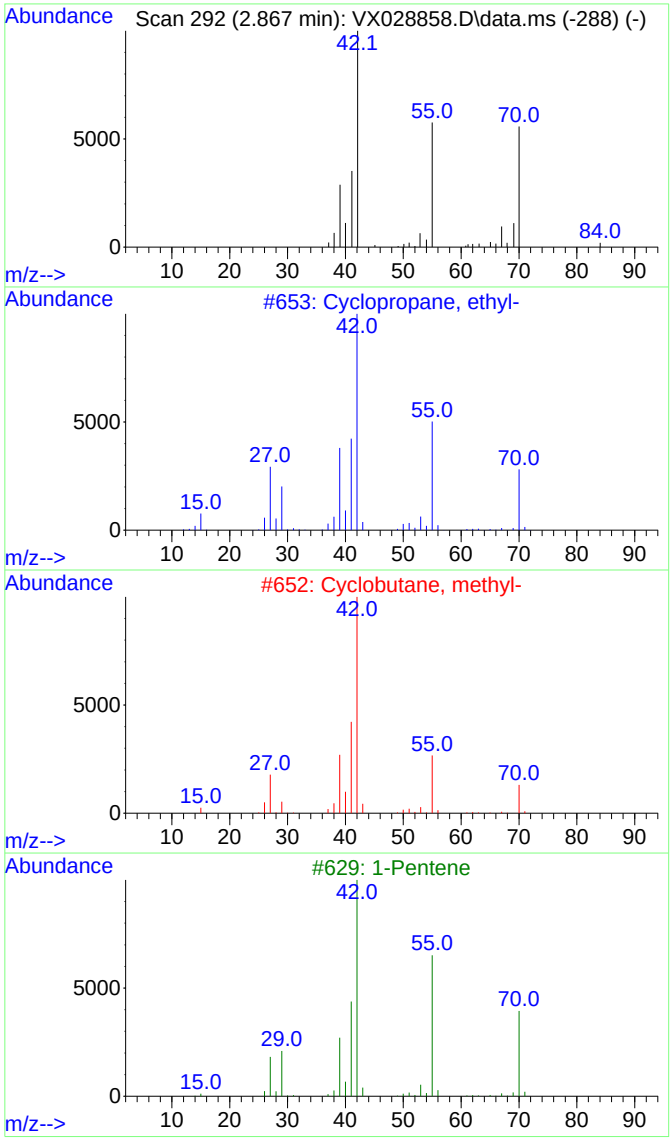
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

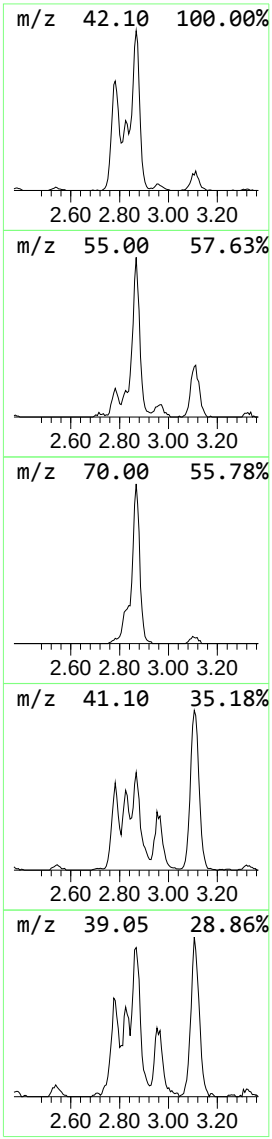
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Cyclopropane, ethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.867	10.59 ug/l	140722	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropane, ethyl-	70	C5H10	001191-96-4	72
2	Cyclobutane, methyl-	70	C5H10	000598-61-8	64
3	1-Pentene	70	C5H10	000109-67-1	64
4	2-Pentene	70	C5H10	000109-68-2	38
5	2H-Tetrazole, 2,5-dimethyl-	98	C3H6N4	004135-93-7	38





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ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-22

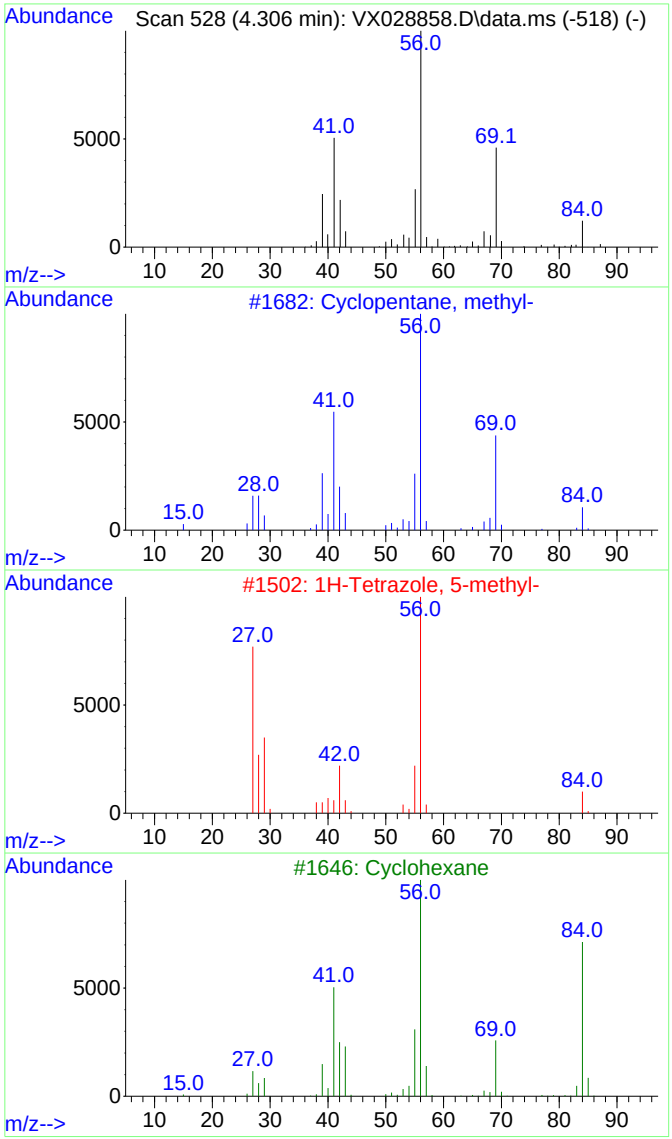
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

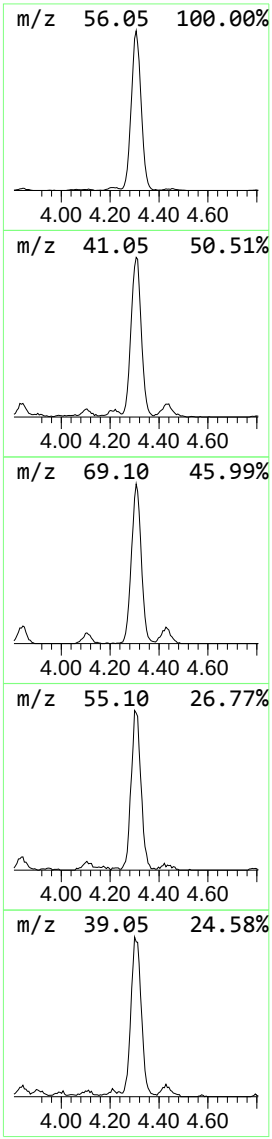
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Cyclopentane, methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.306	35.84 ug/l	476305	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
3	Cyclohexane	84	C6H12	000110-82-7	72
4	Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
5	Cyclobutane	56	C4H8	000287-23-0	50





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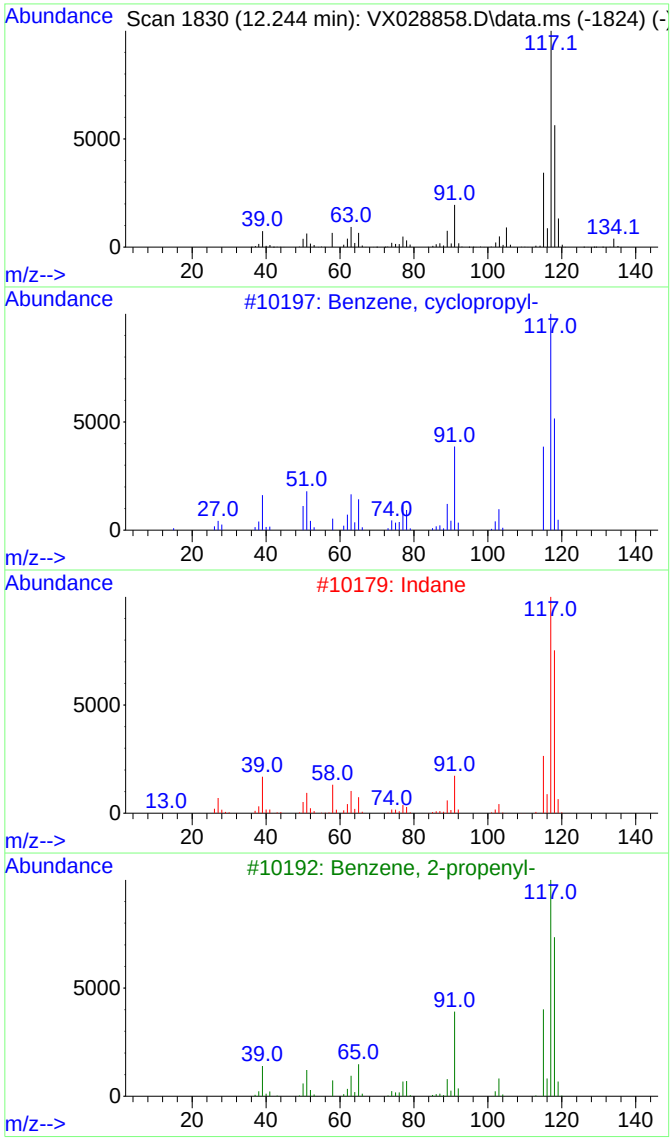
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

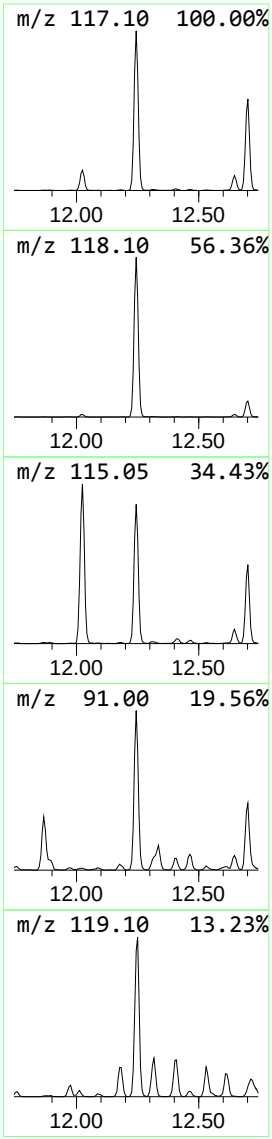
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzene, cyclopropyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	43.45 ug/l	1073150	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, cyclopropyl-	118	C9H10	000873-49-4	76
2	Indane	118	C9H10	000496-11-7	76
3	Benzene, 2-propenyl-	118	C9H10	000300-57-2	76
4	Benzene, 1,1'-(1-ethenyl-1,3-pro...	222	C17H18	061141-97-7	64
5	1,4:5,8-Dimethanobiphenylene, 1,...	184	C14H16	001624-13-1	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052022\
Data File : VX028858.D
Acq On : 20 May 2022 18:06
Operator : JC/MD
Sample : N2943-16
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-22

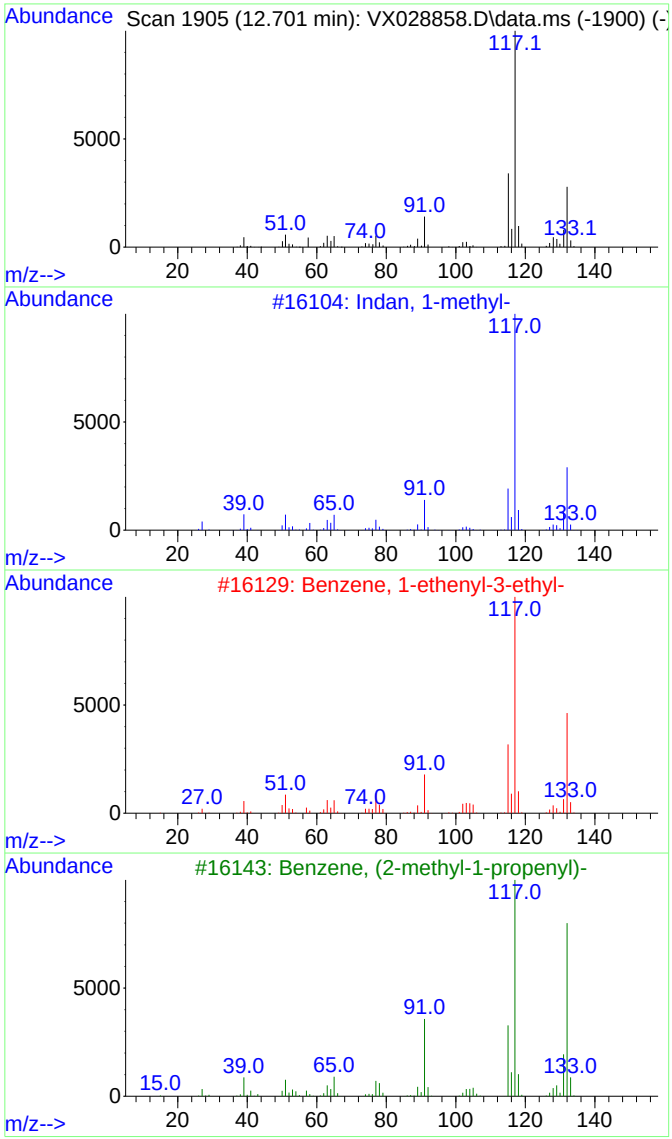
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

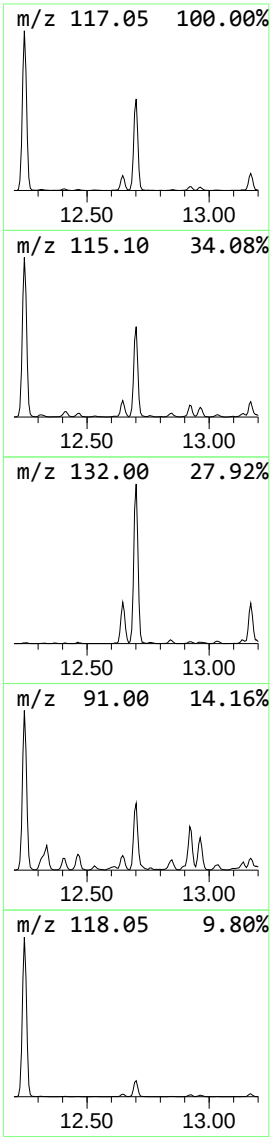
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Indan, 1-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.701	20.65 ug/l	510165	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indan, 1-methyl-	132	C10H12	000767-58-8	93
2	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	91
3	Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	90
4	1-Phenyl-1-butene	132	C10H12	000824-90-8	90
5	1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	86





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052022\
Data File : VX028858.D
Acq On : 20 May 2022 18:06
Operator : JC/MD
Sample : N2943-16
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-22

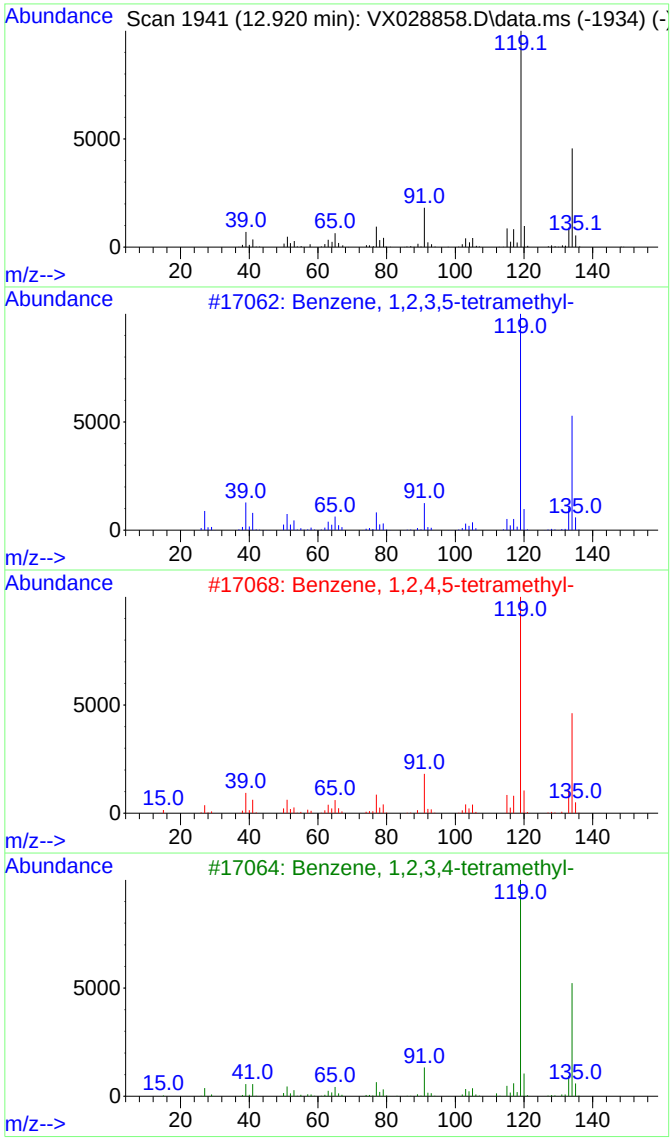
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

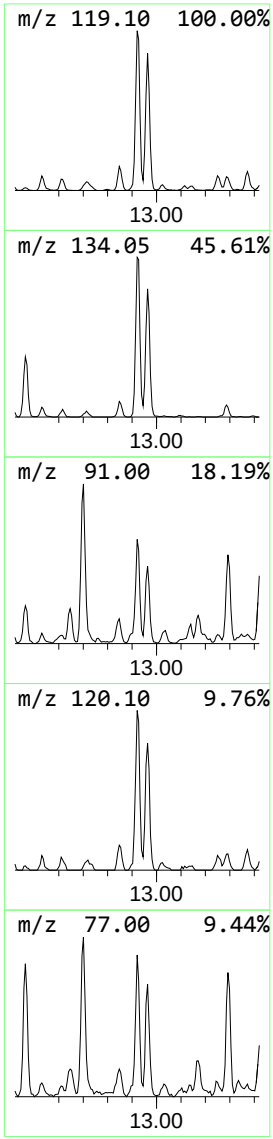
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, 1,2,3,5-tetramethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.921	11.67 ug/l	288267	1,4-Dichlorobenzene-d4	12.024

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





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052022\
Data File : VX028858.D
Acq On : 20 May 2022 18:06
Operator : JC/MD
Sample : N2943-16
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-22

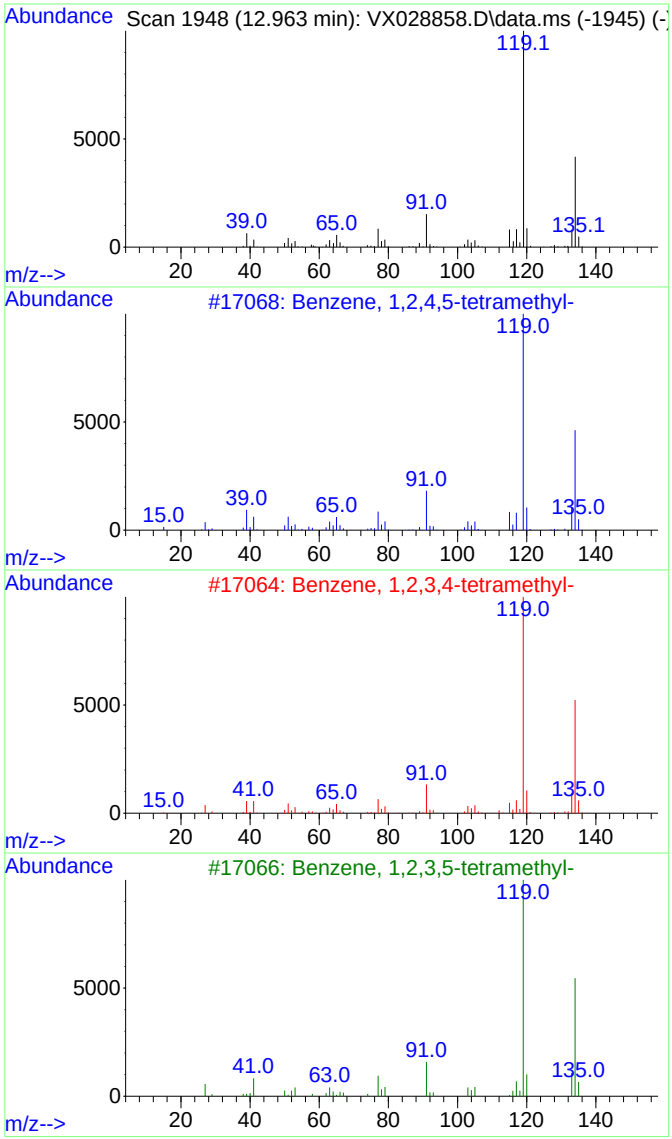
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

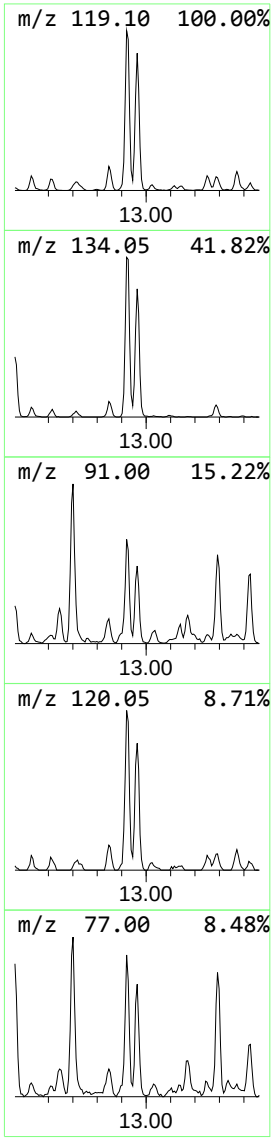
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.963	8.52 ug/l	210504	1,4-Dichlorobenzene-d4	12.024

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	96
4	o-Cymene	134	C10H14	000527-84-4	95
5	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	94





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Data File : VX028858.D
Acq On : 20 May 2022 18:06
Operator : JC/MD
Sample : N2943-16
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-22

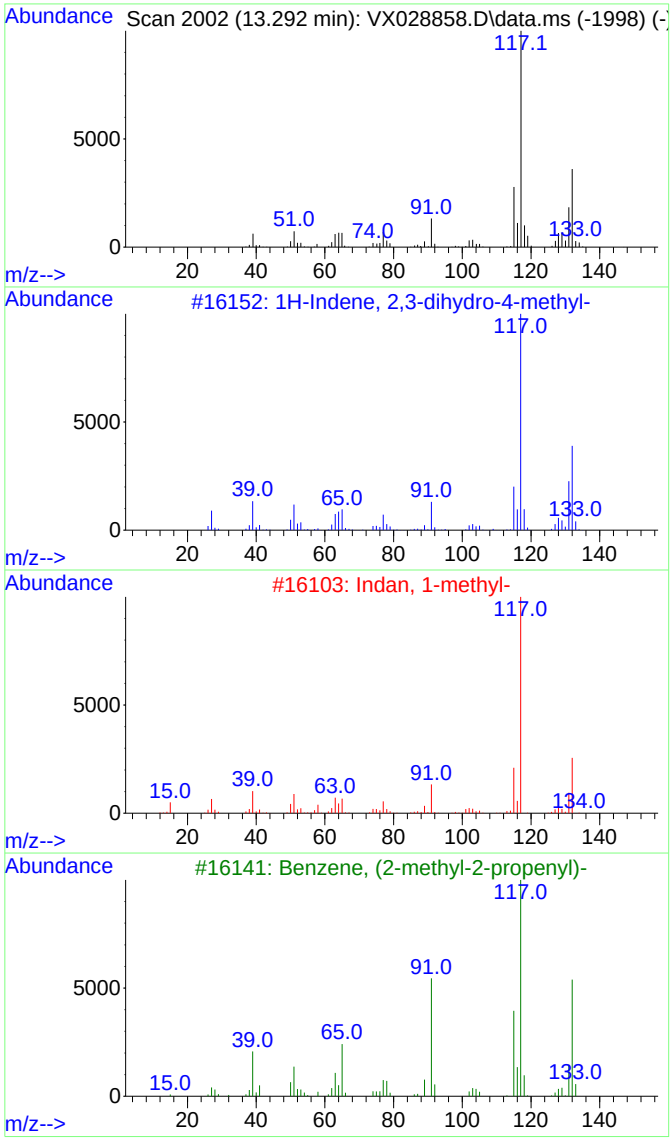
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

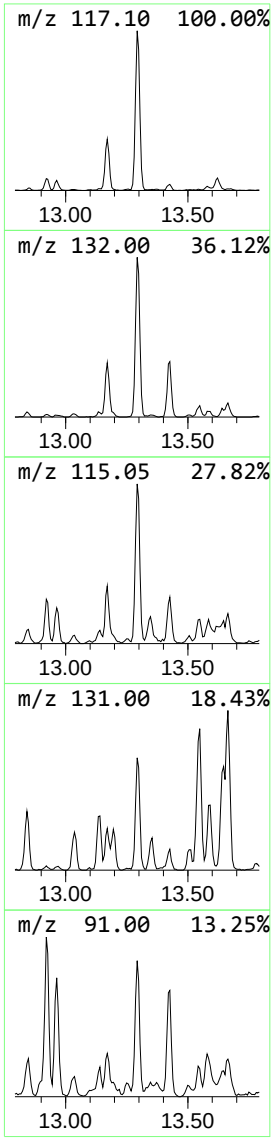
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 1H-Indene, 2,3-dihydro-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	14.37 ug/l	354849	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	87
2	Indan, 1-methyl-	132	C10H12	000767-58-8	87
3	Benzene, (2-methyl-2-propenyl)-	132	C10H12	003290-53-7	86
4	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	86
5	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	83





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052022\
Data File : VX028858.D
Acq On : 20 May 2022 18:06
Operator : JC/MD
Sample : N2943-16
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-22

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Aminomethanesul...	1.264	15.9	ug/l	210611	1	5.556	664436	50.0
Butane, 2-methyl-	1.752	27.0	ug/l	358805	1	5.556	664436	50.0
Butane, 2,3-dim...	2.782	9.8	ug/l	129597	1	5.556	664436	50.0
Cyclopropane, e...	2.867	10.6	ug/l	140722	1	5.556	664436	50.0
Cyclopentane, m...	4.306	35.8	ug/l	476305	1	5.556	664436	50.0
Benzene, cyclop...	12.244	43.5	ug/l	1073150	4	12.024	1234990	50.0
Indan, 1-methyl-	12.701	20.6	ug/l	510165	4	12.024	1234990	50.0
Benzene, 1,2,3,...	12.921	11.7	ug/l	288267	4	12.024	1234990	50.0
Benzene, 1,2,4,...	12.963	8.5	ug/l	210504	4	12.024	1234990	50.0
1H-Indene, 2,3-...	13.292	14.4	ug/l	354849	4	12.024	1234990	50.0