LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120221\
Data File : VX025435.D
Acq On : 02 Dec 2021 17:53
Operator : JC/MD
Sample : M4917-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 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\82X111721W.M
Title : SW846 8260

Signal : TIC: VX025435.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.239	21	25	42	rBV	289994	418324	79.14%	7.570%
2	1.367	43	46	49	rVB	7856	9163	1.73%	0.166%
3	1.745	104	108	124	rVB	44554	69310	13.11%	1.254%
4	1.953	138	142	151	rVB3	9095	15325	2.90%	0.277%
5	2.209	180	184	192	rVB2	6393	10414	1.97%	0.188%
6	2.380	209	212	220	rVB	3641	6070	1.15%	0.110%
7	2.538	230	238	247	rBV	10691	19582	3.70%	0.354%
8	2.782	268	278	282	rBV2	6687	17358	3.28%	0.314%
9	2.825	282	285	288	rVV3	6294	12194	2.31%	0.221%
10	2.867	288	292	301	rVV3	14233	29920	5.66%	0.541%
11	2.965	301	308	323	rVB	23388	50907	9.63%	0.921%
12	3.117	323	333	347	rVB3	31302	79315	15.01%	1.435%
13	3.763	426	439	445	rBV4	4971	17555	3.32%	0.318%
14	4.306	518	528	541	rVV2	34945	101938	19.29%	1.845%
15	4.434	541	549	557	rVB5	3183	8823	1.67%	0.160%
16	5.196	666	674	687	rVB4	3439	10401	1.97%	0.188%
17	5.391	693	706	713	rBV2	63033	181360	34.31%	3.282%
18	5.477	713	720	726	rVV2	31869	98030	18.55%	1.774%
19	5.556	726	733	756	rVB	103866	298729	56.52%	5.406%
20	5.958	790	799	806	rBV	64911	172527	32.64%	3.122%
21	6.043	806	813	825	rVB	75414	200317	37.90%	3.625%
22	6.245	833	846	855	rVB8	4647	22057	4.17%	0.399%
23	6.360	855	865	873	rVB8	3005	10839	2.05%	0.196%
24	6.763	922	931	942	rBV	163722	395624	74.85%	7.159%
25	7.177	990	999	1006	rVB2	6811	14125	2.67%	0.256%
26	7.379	1021	1032	1043	rVB4	10308	27587	5.22%	0.499%
27	7.885	1112	1115	1123	rVV4	4159	7964	1.51%	0.144%
28	8.147	1153	1158	1163	rVB	11803	19855	3.76%	0.359%
29	8.427	1199	1204	1209	rBV	4732	7543	1.43%	0.136%
30	8.506	1211	1217	1224	rVB	14507	23834	4.51%	0.431%
31	8.653	1230	1241	1247	rBV	338085	528563	100.00%	9.565%
32	8.720	1247	1252	1260	rVB	40104	62595	11.84%	1.133%
33	8.958	1287	1291	1298	rVB	13059	20760	3.93%	0.376%
34	9.049	1300	1306	1312	rBV	12646	19332	3.66%	0.350%
35	9.165	1319	1325	1332	rBV	5087	7862	1.49%	0.142%
36	9.457	1365	1373	1377	rBV3	9131	17029	3.22%	0.308%

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Integrator: RTE
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Title : SW846 8260

37	9.945	1448	1453	1461	rBV4	2897	5946	1.12%	0.108%
38	10.055	1465	1471	1477	rBV	341266	453821	85.86%	8.212%
39	10.195	1490	1494	1500	rVB	40213	50367	9.53%	0.911%
40	10.305	1509	1512	1517	rVB	5949	7585	1.44%	0.137%
41	10.963	1615	1620	1626	rBV	65432	81626	15.44%	1.477%
42	11.085	1634	1640	1650	rVB	268697	348925	66.01%	6.314%
43	11.305	1670	1676	1685	rVB	56486	70225	13.29%	1.271%
44	11.616	1722	1727	1733	rVB	17029	21467	4.06%	0.388%
45	11.756	1746	1750	1755	rVB	7183	8704	1.65%	0.158%
46	11.866	1762	1768	1770	rBV	7721	9864	1.87%	0.179%
47	11.890	1770	1772	1778	rVB	8568	9929	1.88%	0.180%
48	12.024	1789	1794	1801	rBV	335293	429439	81.25%	7.771%
49	12.091	1801	1805	1810	rVB	7140	8928	1.69%	0.162%
50	12.244	1823	1830	1837	rBV	202922	249255	47.16%	4.511%
51	12.317	1837	1842	1848	rVB2	8616	13502	2.55%	0.244%
52	12.408	1852	1857	1862	rBV2	12402	14824	2.80%	0.268%
53	12.463	1862	1866	1872	rVB	26365	31190	5.90%	0.564%
54	12.530	1872	1877	1884	rBV	5043	6180	1.17%	0.112%
55	12.615	1884	1891	1893	rBV	6995	9435	1.79%	0.171%
56	12.646	1893	1896	1900	rVV	22496	26352	4.99%	0.477%
57	12.701	1900	1905	1912	rVB	105913	130505	24.69%	2.362%
58	12.847	1924	1929	1934	rVB2	13036	17710	3.35%	0.320%
59	12.926	1934	1942	1945	rVV	49890	68082	12.88%	1.232%
60	12.963	1945	1948	1954	rVB	40789	48628	9.20%	0.880%
61	13.030	1954	1959	1964	rVB2	4716	6495	1.23%	0.118%
62	13.140	1974	1977	1979	rBV2	5587	6252	1.18%	0.113%
63	13.170	1979	1982	1991	rVB2	19504	27080	5.12%	0.490%
64	13.256	1991	1996	1998	rBV2	4176	5373	1.02%	0.097%
65	13.292	1998	2002	2007	rVV	57842	74417	14.08%	1.347%
66	13.347	2007	2011	2019	rVV6	9010	19247	3.64%	0.348%
67	13.426	2019	2024	2028	rVB	25186	32957	6.24%	0.596%
68	13.506	2033	2037	2040	rBV4	3612	5400	1.02%	0.098%
69	13.548	2040	2044	2046	rVV	12039	15568	2.95%	0.282%
70	13.579	2046	2049	2056	rVV2	16180	32341	6.12%	0.585%
71	13.646	2056	2060	2061	rVV2	8237	12094	2.29%	0.219%
72	13.664	2061	2063	2070	rVB2	11177	16415	3.11%	0.297%
73	13.780	2074	2082	2090	rBV	26618	38183	7.22%	0.691%
74	13.859	2090	2095	2101	rVB2	5529	9344	1.77%	0.169%
75	13.926	2101	2106	2111	rBV2	7996	11390	2.15%	0.206%
76	14.079	2126	2131	2134	rBV	5578	6752	1.28%	0.122%

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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
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Title : SW846 8260

77	14.213	2149	2153	2165	rBV2	17202	27074	5.12%	0.490%
78	14.322	2167	2171	2176	rVV	5066	6249	1.18%	0.113%
79	14.377	2176	2180	2184	rVB	5534	7436	1.41%	0.135%
80	14.780	2242	2246	2255	rBV	18093	24510	4.64%	0.444%
81	15.121	2297	2302	2306	rBV2	4419	5824	1.10%	0.105%

Sum of corrected areas: 5526021

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Instrument :
MSVOA_X
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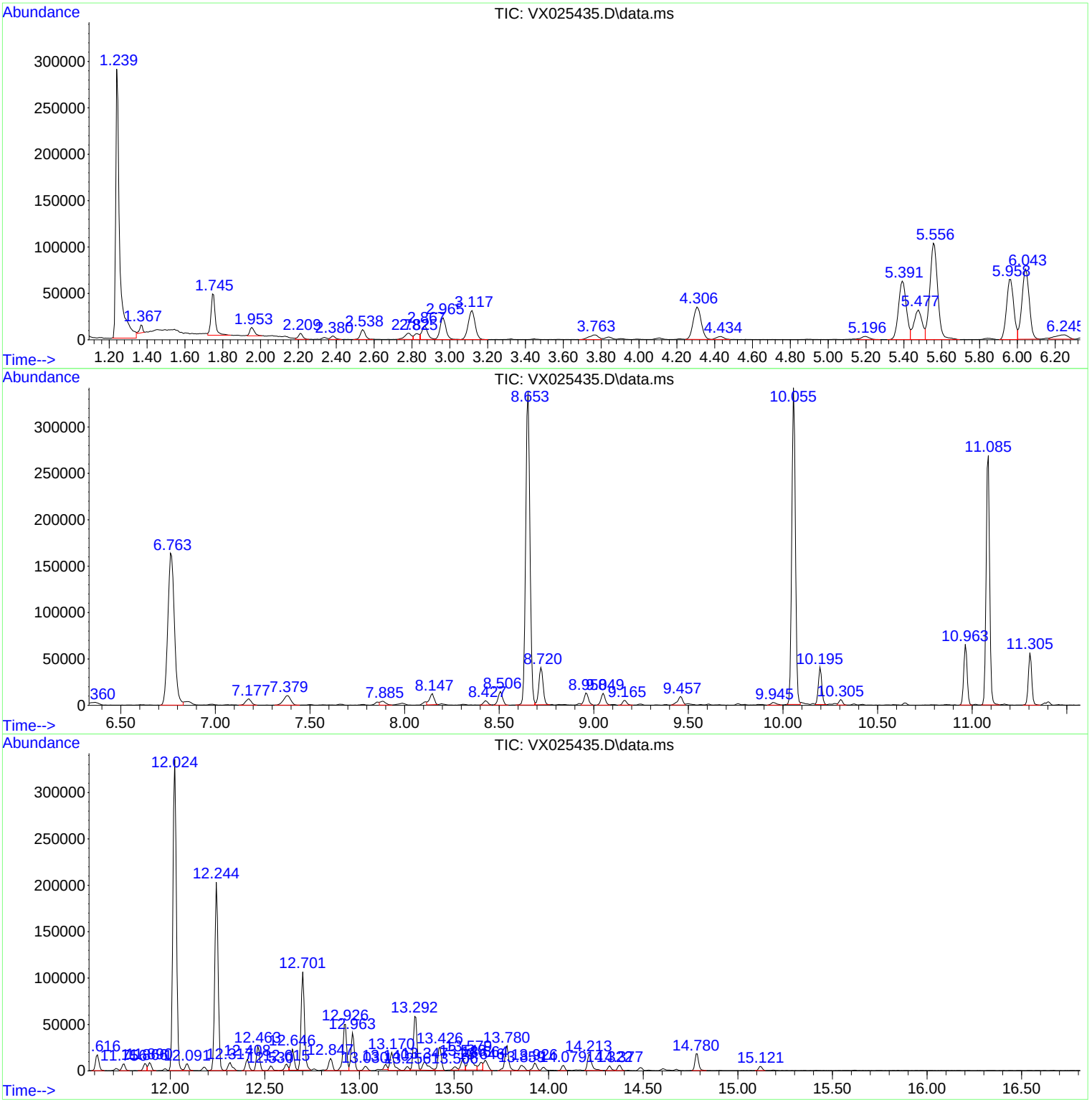
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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



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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

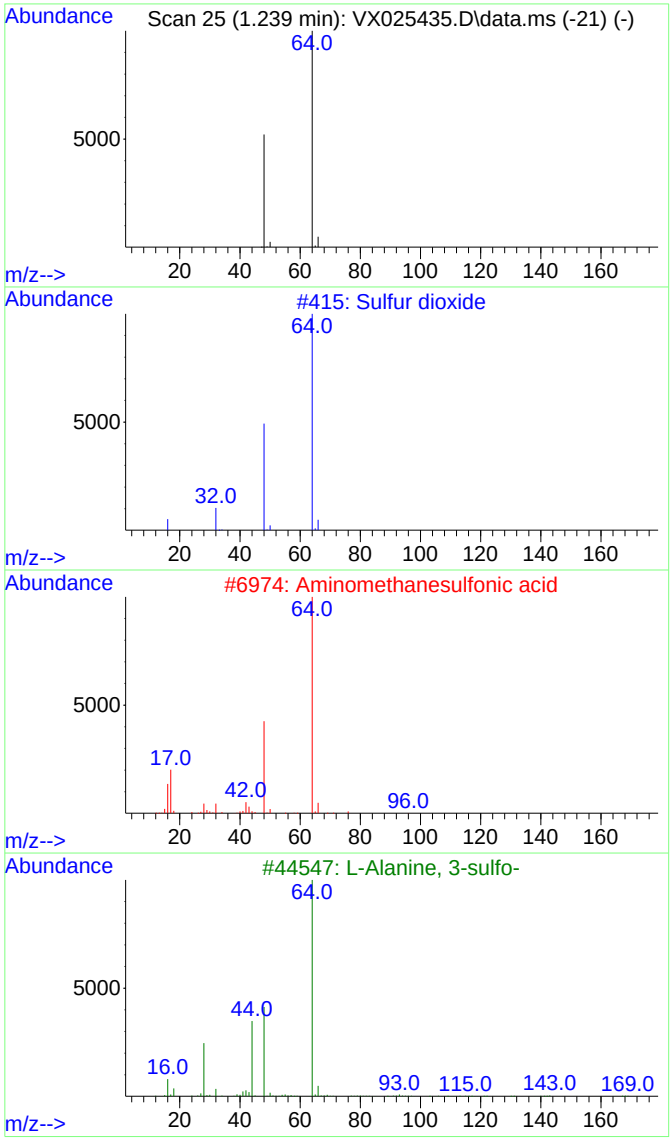
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

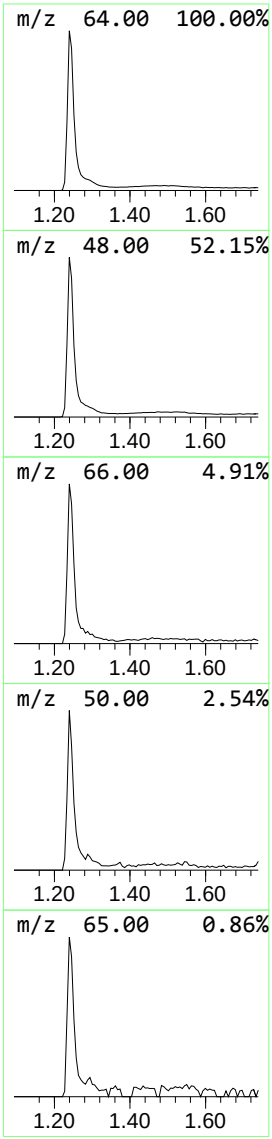
****

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.239	70.02 ug/l	418324	Pentafluorobenzene	5.556

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





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ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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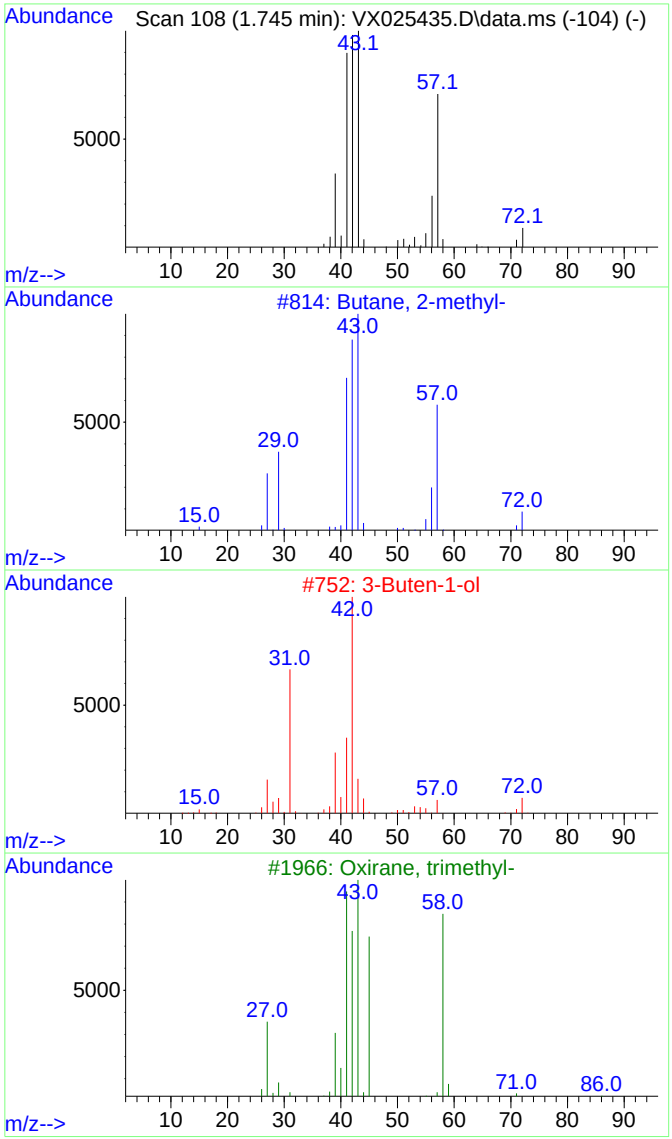
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

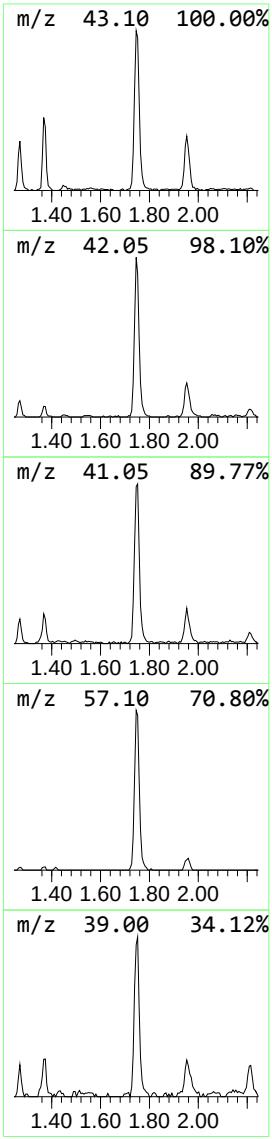
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.745	11.60 ug/l	69310	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	90
2	3-Buten-1-ol	72	C4H8O	000627-27-0	43
3	Oxirane, trimethyl-	86	C5H10O	005076-19-7	38
4	Pentane	72	C5H12	000109-66-0	36
5	2(3H)-Furanone, dihydro-4-methyl-	100	C5H8O2	001679-49-8	28





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ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-22

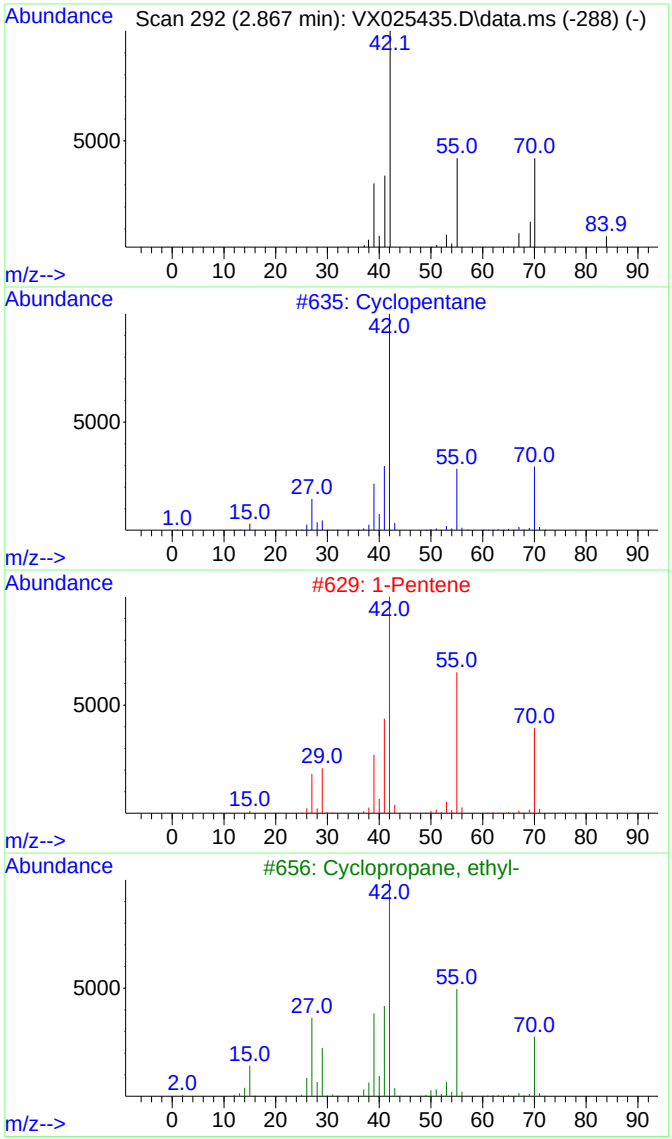
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

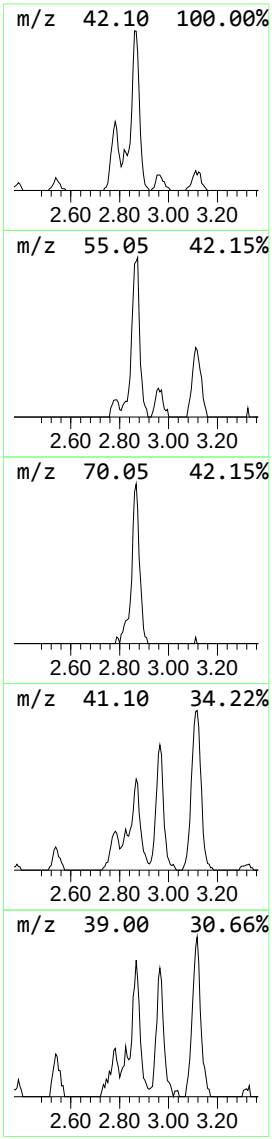
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Cyclopentane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.867	5.01 ug/l	29920	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane	70	C5H10	000287-92-3	72
2	1-Pentene	70	C5H10	000109-67-1	64
3	Cyclopropane, ethyl-	70	C5H10	001191-96-4	53
4	Cyclobutanone	70	C4H6O	001191-95-3	9
5	Cyclobutane, methyl-	70	C5H10	000598-61-8	9





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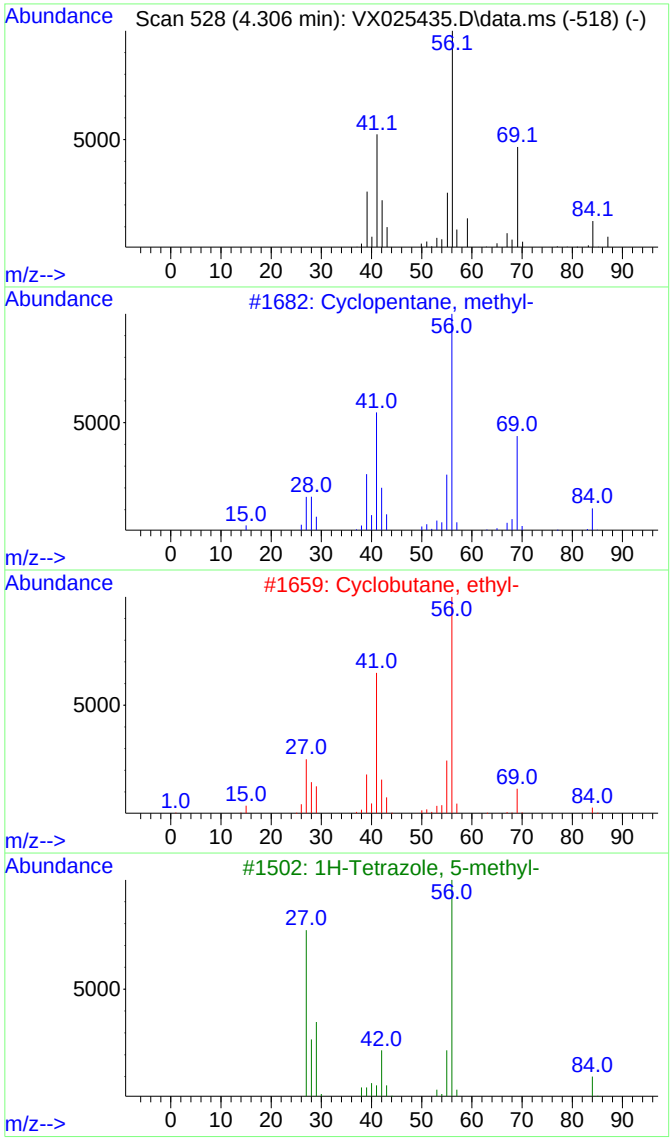
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

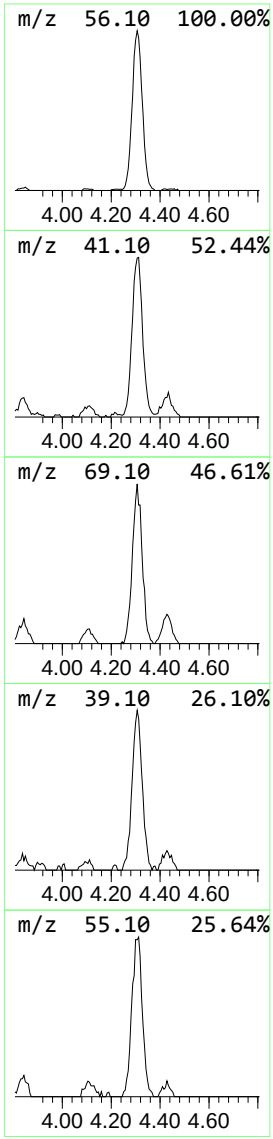
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Cyclopentane, methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.306	17.06 ug/l	101938	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	87
2	Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
3	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	59
4	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	45
5	Cyclohexane	84	C6H12	000110-82-7	38





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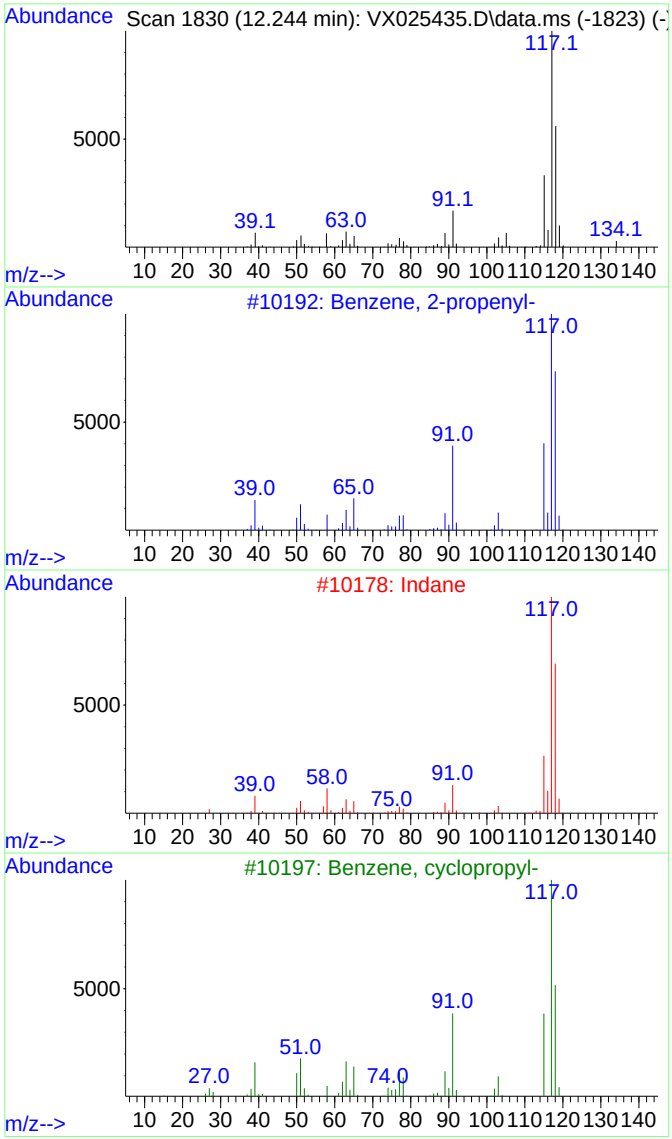
Quant Title : SW846 8260

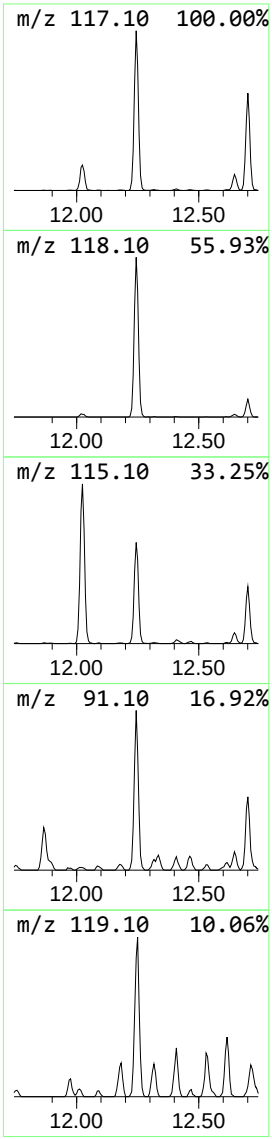
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Benzene, 2-propenyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	29.02 ug/l	249255	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-propenyl-	118	C9H10	000300-57-2	87
2	Indane	118	C9H10	000496-11-7	87
3	Benzene, cyclopropyl-	118	C9H10	000873-49-4	81
4	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	64
5	Deltacyclene	118	C9H10	007785-10-6	53





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ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-22

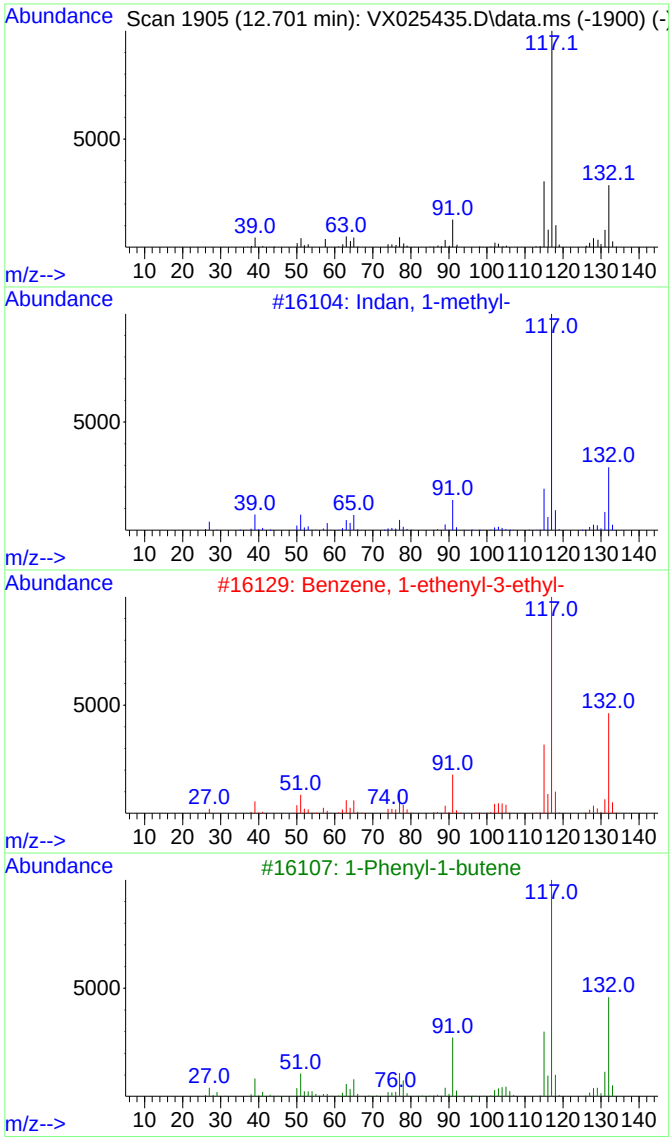
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

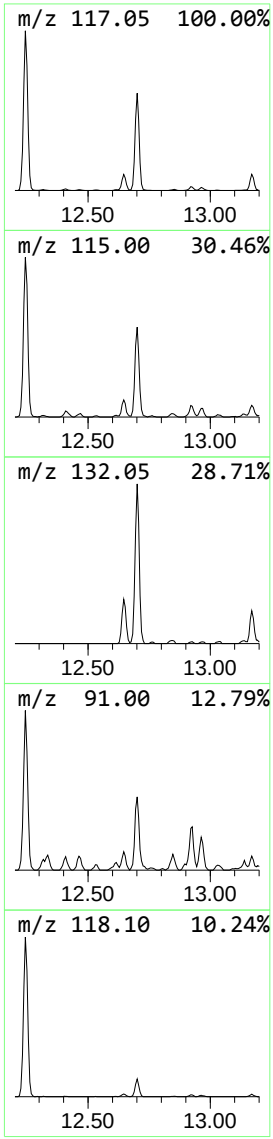
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Indan, 1-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.701	15.19 ug/l	130505	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	1-Phenyl-1-butene	132	C10H12	000824-90-8	87
4	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	86
5	1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	86





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120221\
Data File : VX025435.D
Acq On : 02 Dec 2021 17:53
Operator : JC/MD
Sample : M4917-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-22

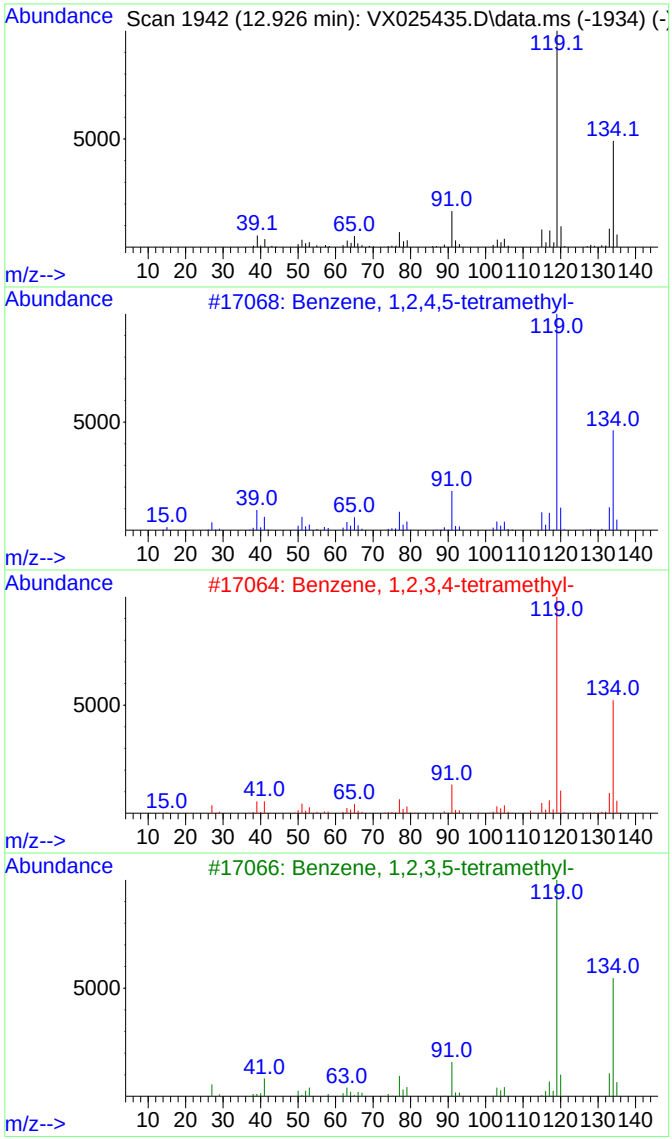
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

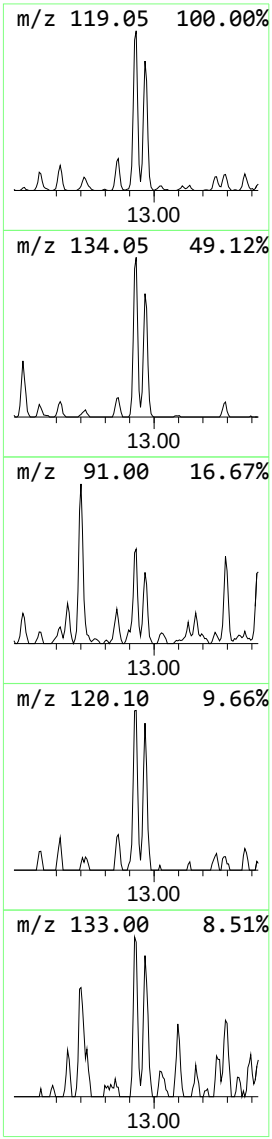
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.926	7.93 ug/l	68082	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	97
4	Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	91
5	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	91





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Data File : VX025435.D
Acq On : 02 Dec 2021 17:53
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Sample : M4917-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-22

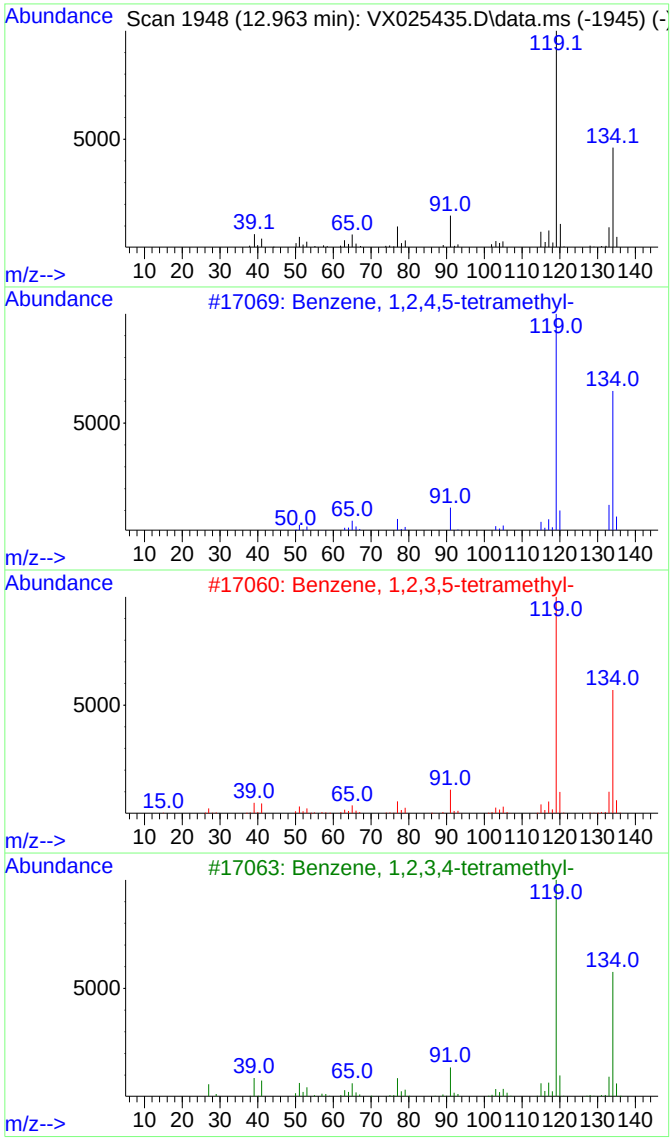
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

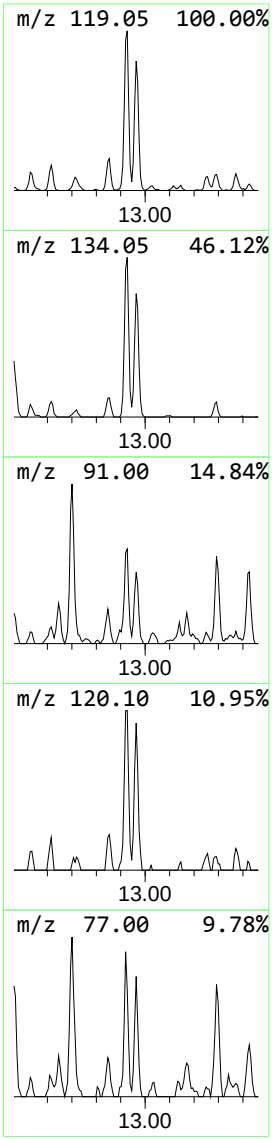
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.963	5.66 ug/l	48628	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	94
2	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	94
3	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	94
4	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	94
5	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	93





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120221\
Data File : VX025435.D
Acq On : 02 Dec 2021 17:53
Operator : JC/MD
Sample : M4917-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-22

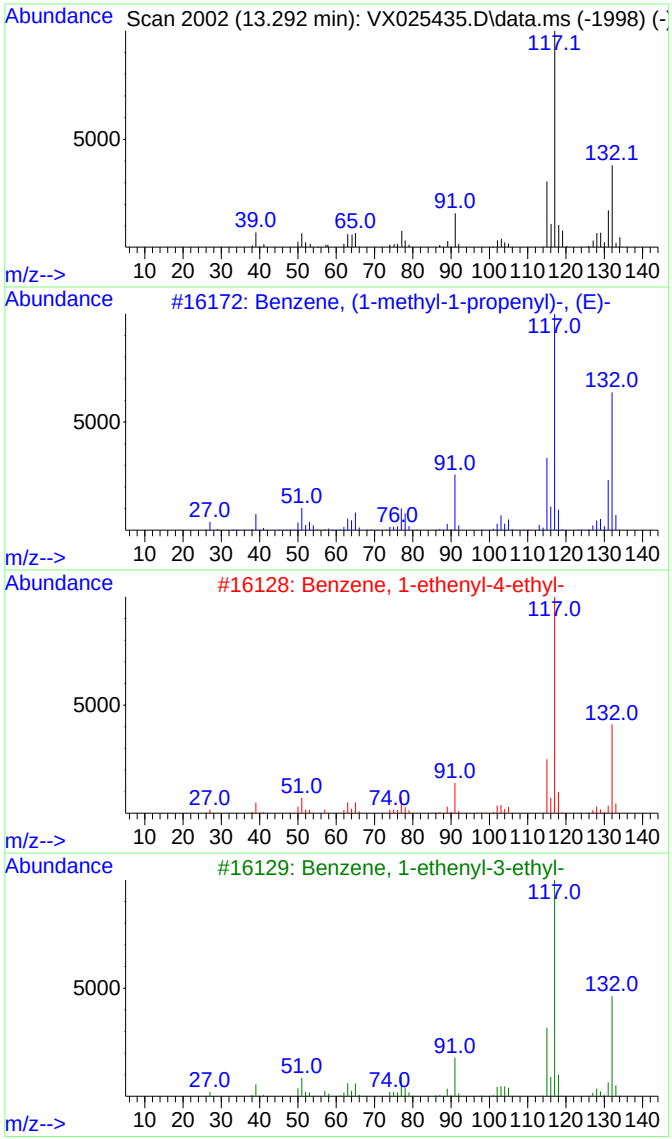
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

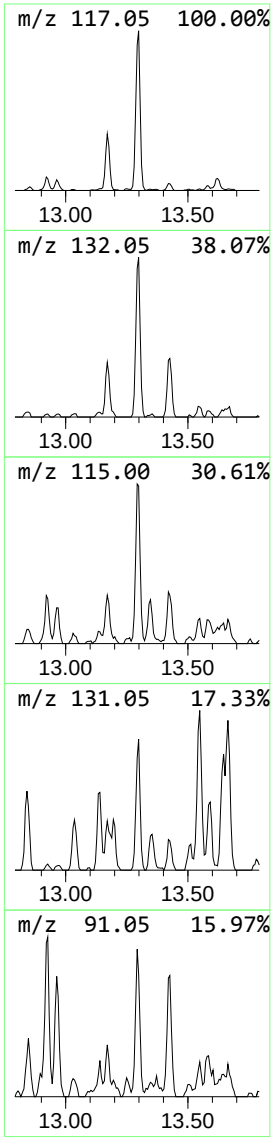
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, (1-methyl-1-propen... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	8.66 ug/l	74417	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	91
2	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	91
3	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	87
4	3-Phenylbut-1-ene	132	C10H12	000934-10-1	87
5	Benzene, 2-butenyl-	132	C10H12	001560-06-1	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120221\
Data File : VX025435.D
Acq On : 02 Dec 2021 17:53
Operator : JC/MD
Sample : M4917-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-22

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.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
Sulfur dioxide	1.239	70.0	ug/l	418324	1	5.556	298729	50.0
Butane, 2-methyl-	1.745	11.6	ug/l	69310	1	5.556	298729	50.0
Cyclopentane	2.867	5.0	ug/l	29920	1	5.556	298729	50.0
Cyclopentane, m...	4.306	17.1	ug/l	101938	1	5.556	298729	50.0
Benzene, 2-prop...	12.244	29.0	ug/l	249255	4	12.024	429439	50.0
Indan, 1-methyl-	12.701	15.2	ug/l	130505	4	12.024	429439	50.0
Benzene, 1,2,4,...	12.926	7.9	ug/l	68082	4	12.024	429439	50.0
Benzene, 1,2,3,...	12.963	5.7	ug/l	48628	4	12.024	429439	50.0
Benzene, (1-met...	13.292	8.7	ug/l	74417	4	12.024	429439	50.0