LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052022\
Data File : VX028856.D
Acq On : 20 May 2022 17:19
Operator : JC/MD
Sample : N2943-14
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-32

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: VX028856.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.258	20	28	44	rBV	37899	125003	7.45%	0.913%
2	1.752	104	109	115	rBV2	12275	18777	1.12%	0.137%
3	2.532	230	237	250	rBV	16536	33421	1.99%	0.244%
4	2.953	299	306	319	rVB2	16608	41851	2.49%	0.306%
5	3.111	319	332	342	rBV2	21672	52558	3.13%	0.384%
6	3.757	428	438	447	rBV4	8872	26508	1.58%	0.194%
7	4.306	519	528	539	rVB4	10324	31131	1.85%	0.227%
8	5.391	694	706	718	rBV	158017	463844	27.63%	3.388%
9	5.556	722	733	759	rVB	258762	762672	45.43%	5.570%
10	5.958	789	799	809	rBV	172083	460273	27.42%	3.361%
11	6.257	833	848	857	rVB	13355	46956	2.80%	0.343%
12	6.763	922	931	942	rBV	418866	991836	59.09%	7.244%
13	7.372	1023	1031	1041	rVB8	9643	27626	1.65%	0.202%
14	7.988	1124	1132	1139	rVB2	13875	27237	1.62%	0.199%
15	8.110	1144	1152	1156	rBV	23375	49618	2.96%	0.362%
16	8.653	1234	1241	1249	rBV	847576	1340199	79.84%	9.788%
17	8.958	1279	1291	1300	rVB4	17612	33379	1.99%	0.244%
18	9.049	1300	1306	1311	rBV2	11424	18719	1.12%	0.137%
19	10.055	1465	1471	1481	rBV	895812	1168913	69.64%	8.537%
20	10.195	1488	1494	1505	rVV	518919	657526	39.17%	4.802%
21	10.305	1507	1512	1520	rVB	177549	227537	13.55%	1.662%
22	10.646	1563	1568	1575	rVB	24404	32888	1.96%	0.240%
23	10.963	1615	1620	1626	rVB	47318	59100	3.52%	0.432%
24	11.085	1634	1640	1654	rBV	682752	887830	52.89%	6.484%
25	11.305	1671	1676	1684	rVB	125336	150777	8.98%	1.101%
26	11.402	1684	1692	1697	rVV	101788	137546	8.19%	1.005%
27	11.616	1721	1727	1736	rBV	117023	148678	8.86%	1.086%
28	11.750	1744	1749	1757	rBV	1346546	1678625	100.00%	12.259%
29	12.024	1789	1794	1800	rBV	1068197	1324443	78.90%	9.673%
30	12.085	1800	1804	1810	rVB	307180	395795	23.58%	2.891%
31	12.244	1823	1830	1837	rBV	473314	593546	35.36%	4.335%
32	12.311	1837	1841	1850	rVB3	39594	67594	4.03%	0.494%
33	12.408	1852	1857	1862	rBV2	26746	38058	2.27%	0.278%
34	12.463	1862	1866	1873	rVB	35220	43690	2.60%	0.319%
35	12.530	1873	1877	1879	rBV	61017	74391	4.43%	0.543%
36	12.554	1879	1881	1886	rVB	48060	52951	3.15%	0.387%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052022\
Data File : VX028856.D
Acq On : 20 May 2022 17:19
Operator : JC/MD
Sample : N2943-14
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-32

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	12.615	1886	1891	1894	rBV	104736	123155	7.34%	0.899%
38	12.646	1894	1896	1901	rVV	29100	33767	2.01%	0.247%
39	12.701	1901	1905	1913	rVB2	86667	132473	7.89%	0.967%
40	12.847	1925	1929	1934	rVB2	29252	37120	2.21%	0.271%
41	12.920	1934	1941	1945	rBV	67432	89391	5.33%	0.653%
42	12.963	1945	1948	1954	rVV	111551	129562	7.72%	0.946%
43	13.170	1978	1982	1987	rVB	62491	71694	4.27%	0.524%
44	13.292	1998	2002	2007	rVB2	158061	199278	11.87%	1.455%
45	13.426	2019	2024	2031	rVB	50014	69531	4.14%	0.508%
46	13.542	2040	2043	2046	rBV	13130	16796	1.00%	0.123%
47	13.579	2046	2049	2057	rVV4	16710	34832	2.08%	0.254%
48	13.664	2061	2063	2069	rVB3	15318	21802	1.30%	0.159%
49	13.774	2074	2081	2088	rBV	238910	312865	18.64%	2.285%
50	13.865	2091	2096	2101	rVB3	11998	19773	1.18%	0.144%
51	14.073	2126	2130	2138	rBV2	11282	18148	1.08%	0.133%
52	14.219	2149	2154	2164	rBV5	14161	31037	1.85%	0.227%
53	14.780	2241	2246	2252	rBV	45808	59873	3.57%	0.437%

Sum of corrected areas: 13692593

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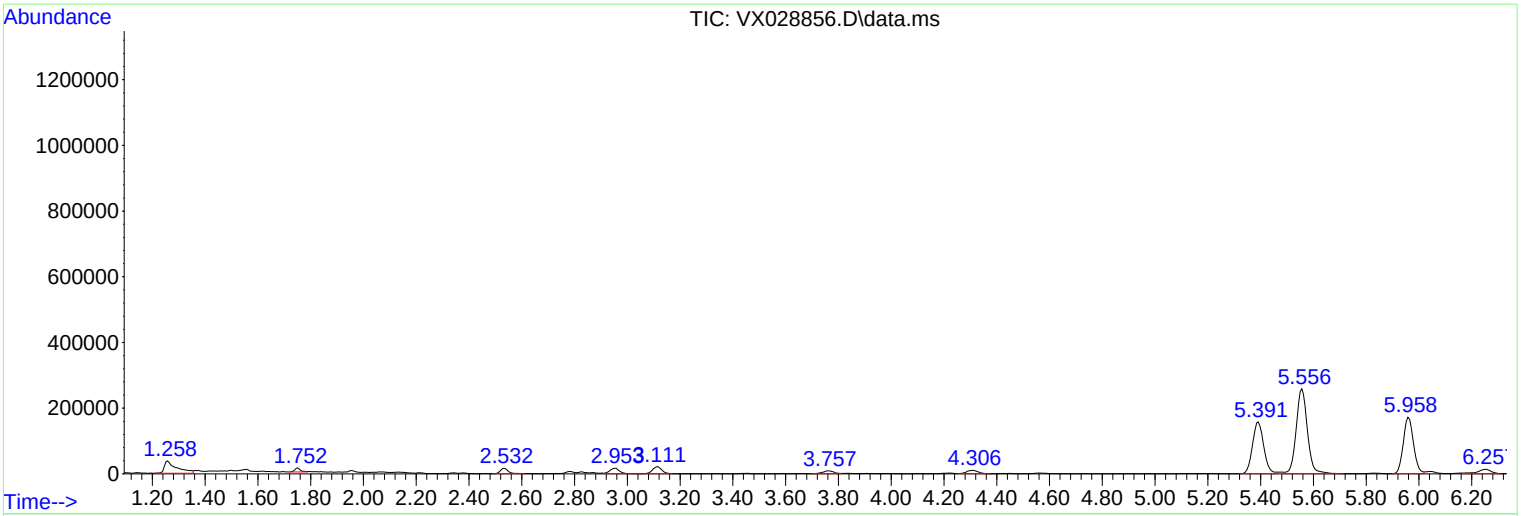
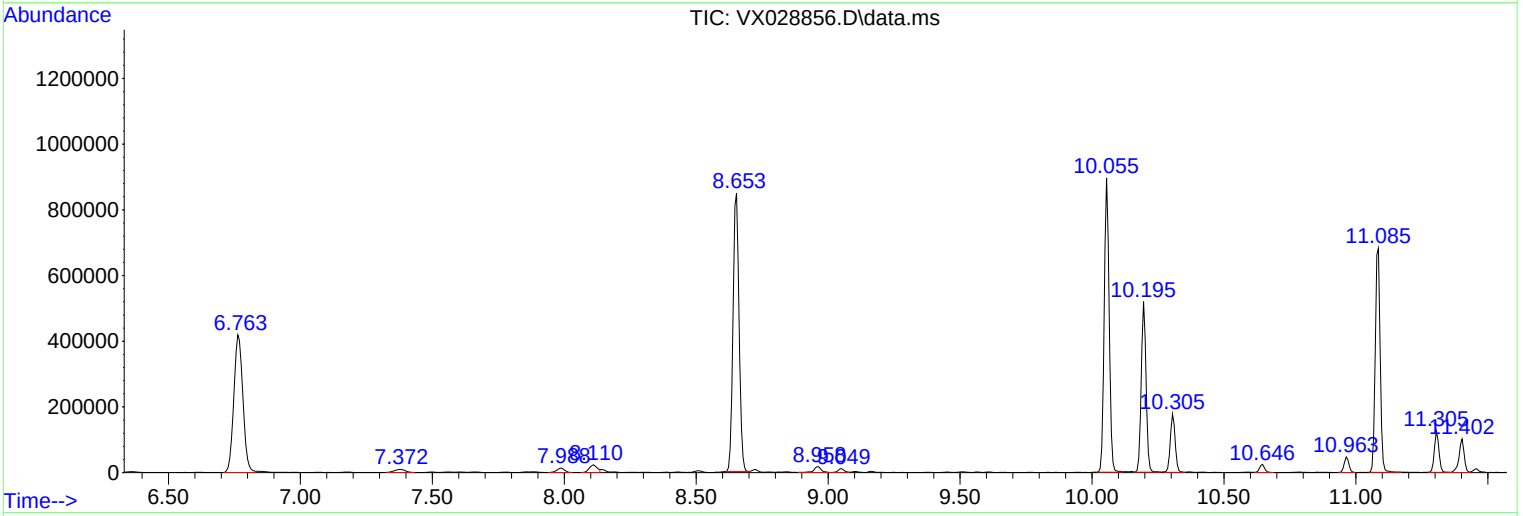
ALS Vial : 16 Sample Multiplier: 1

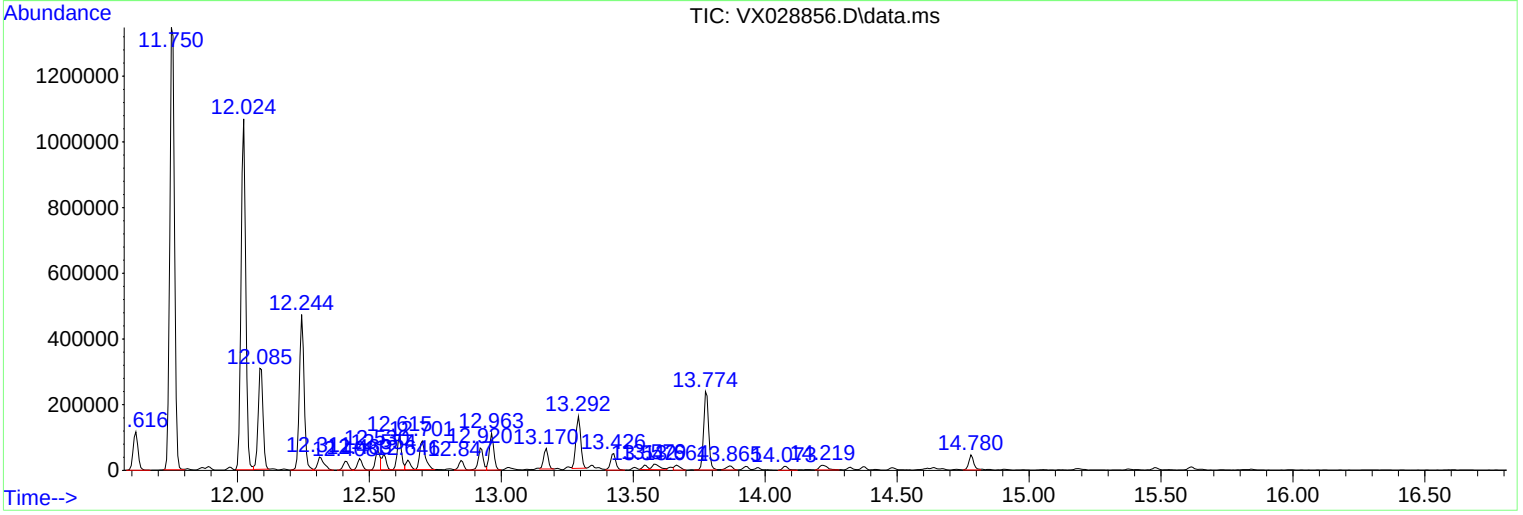
Instrument :
MSVOA_X
ClientSampleId :
MW-32

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







Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052022\
Data File : VX028856.D
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Operator : JC/MD
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ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-32

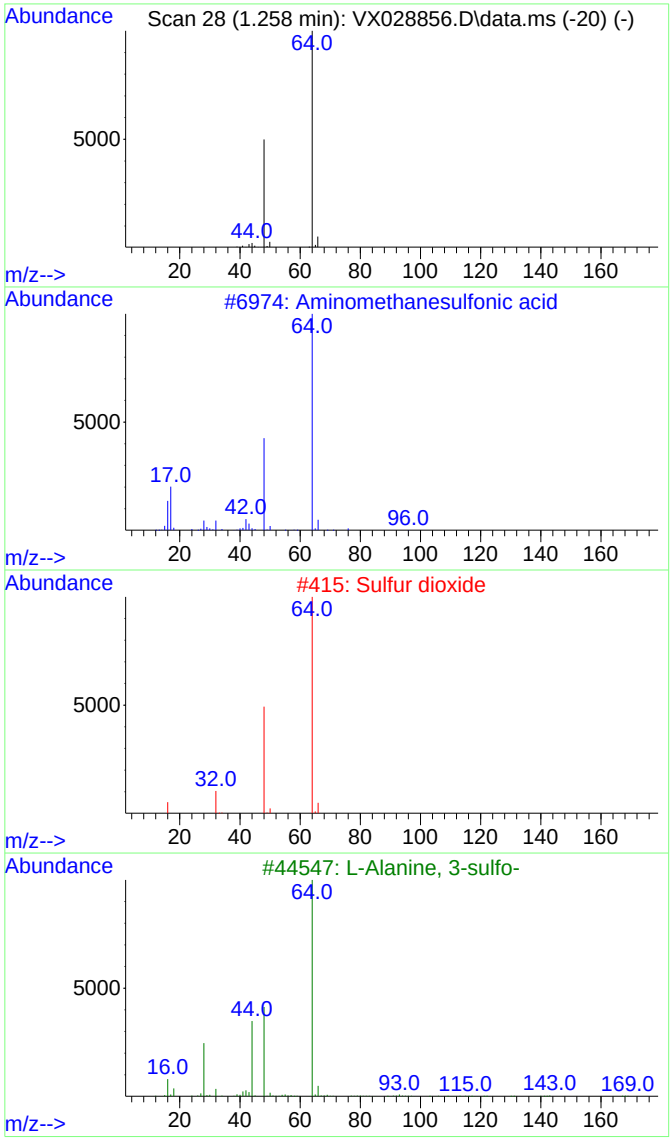
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

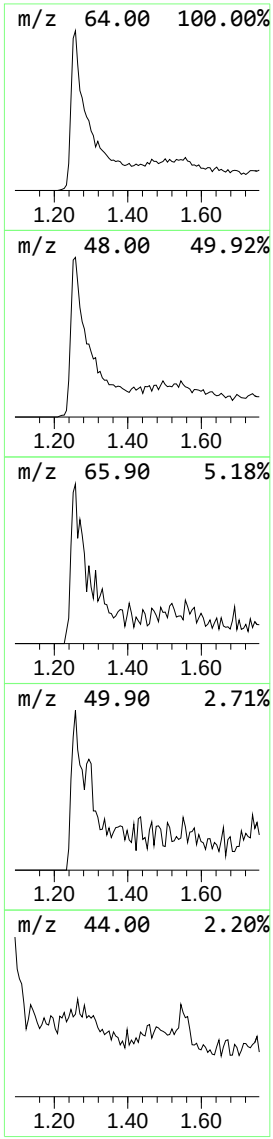
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Aminomethanesulfonic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.258	8.20 ug/l	125003	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	Ethene, 1,2-difluoro-	64	C2H2F2	001691-13-0	4





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052022\
Data File : VX028856.D
Acq On : 20 May 2022 17:19
Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-32

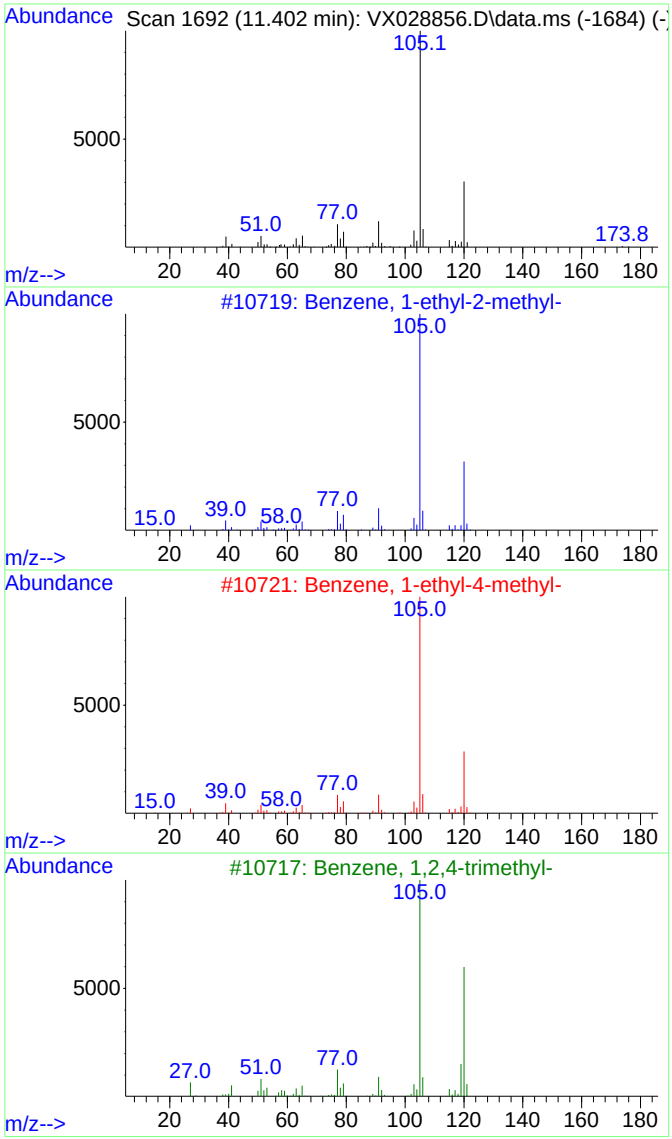
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

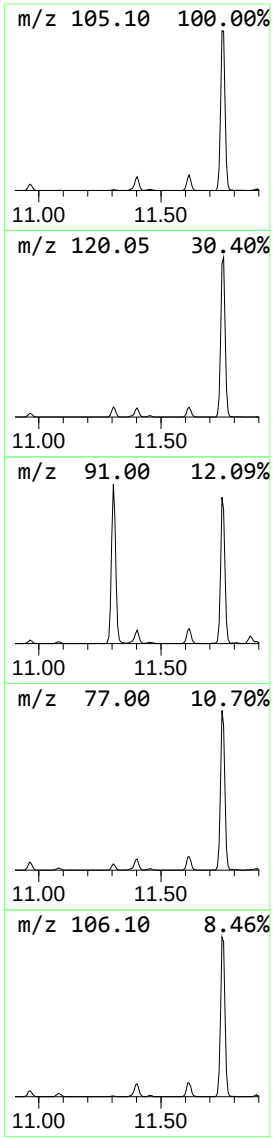
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 unknown5.19 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.402	5.19 ug/l	137546	1,4-Dichlorobenzene-d4	12.024

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-4-methyl-	120	C9H12	000622-96-8	91
3	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	90
5	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052022\
Data File : VX028856.D
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Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-32

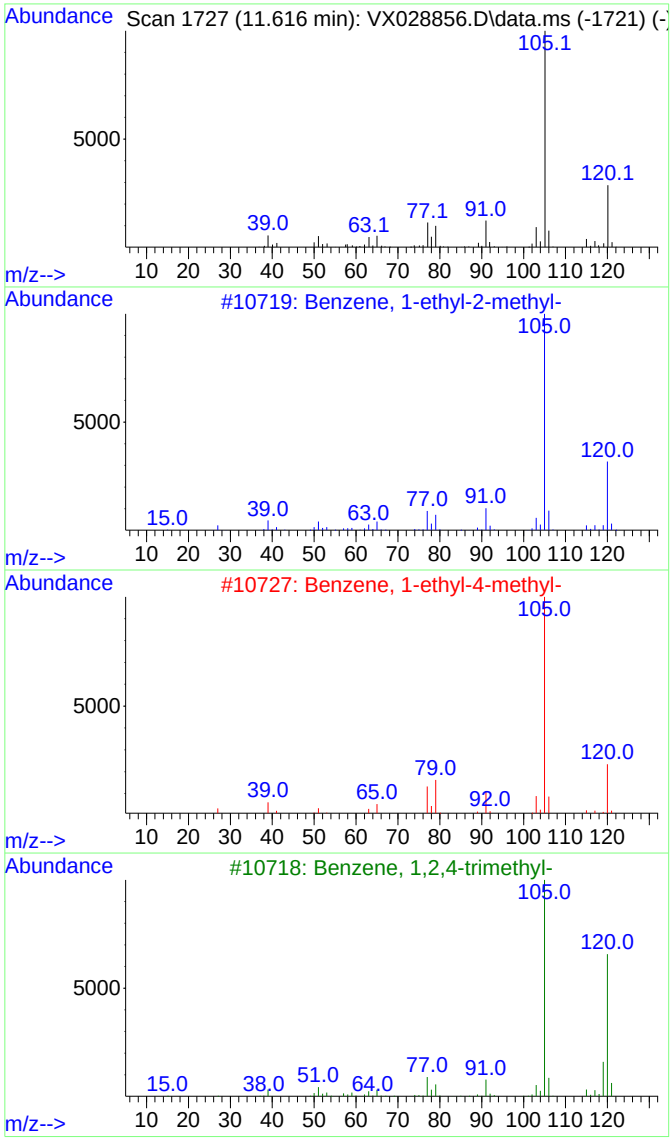
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

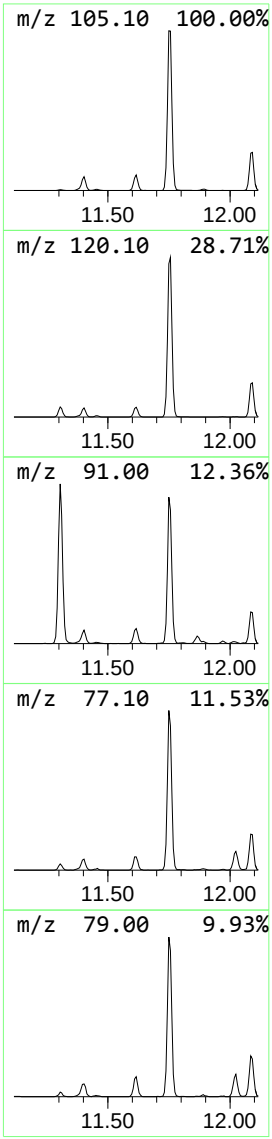
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Benzene, 1-ethyl-4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.616	5.61 ug/l	148678	1,4-Dichlorobenzene-d4	12.024

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-4-methyl-	120	C9H12	000622-96-8	94
3	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5	Mesitylene	120	C9H12	000108-67-8	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052022\
Data File : VX028856.D
Acq On : 20 May 2022 17:19
Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-32

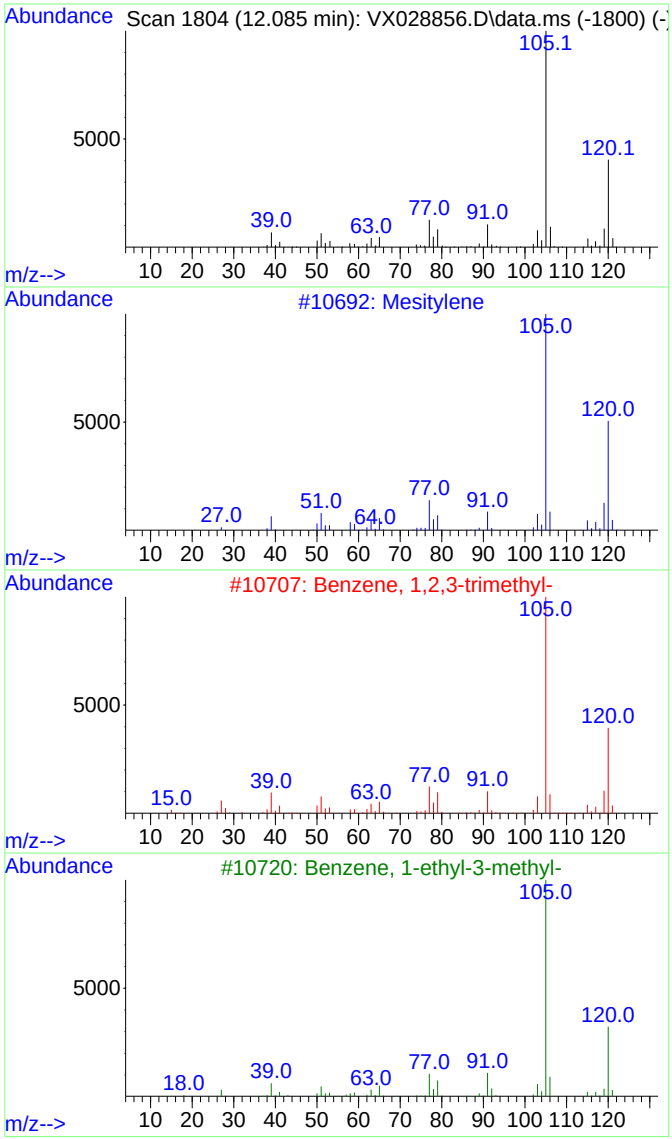
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

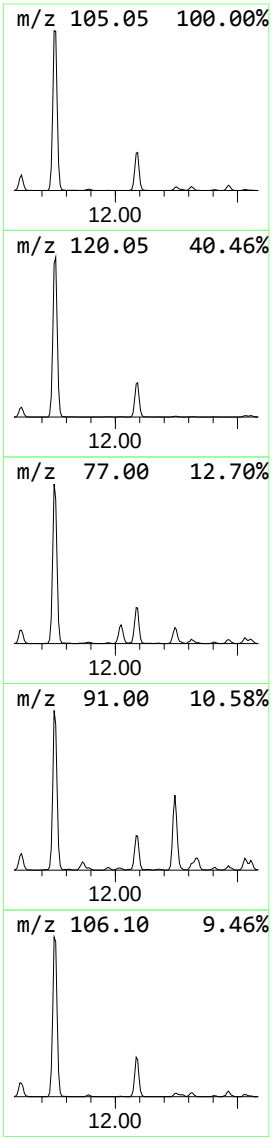
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Benzene, 1,2,3-trimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.085	14.94 ug/l	395795	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Mesitylene	120	C9H12	000108-67-8	97
2	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
3	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
4	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90





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Data File : VX028856.D
Acq On : 20 May 2022 17:19
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ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-32

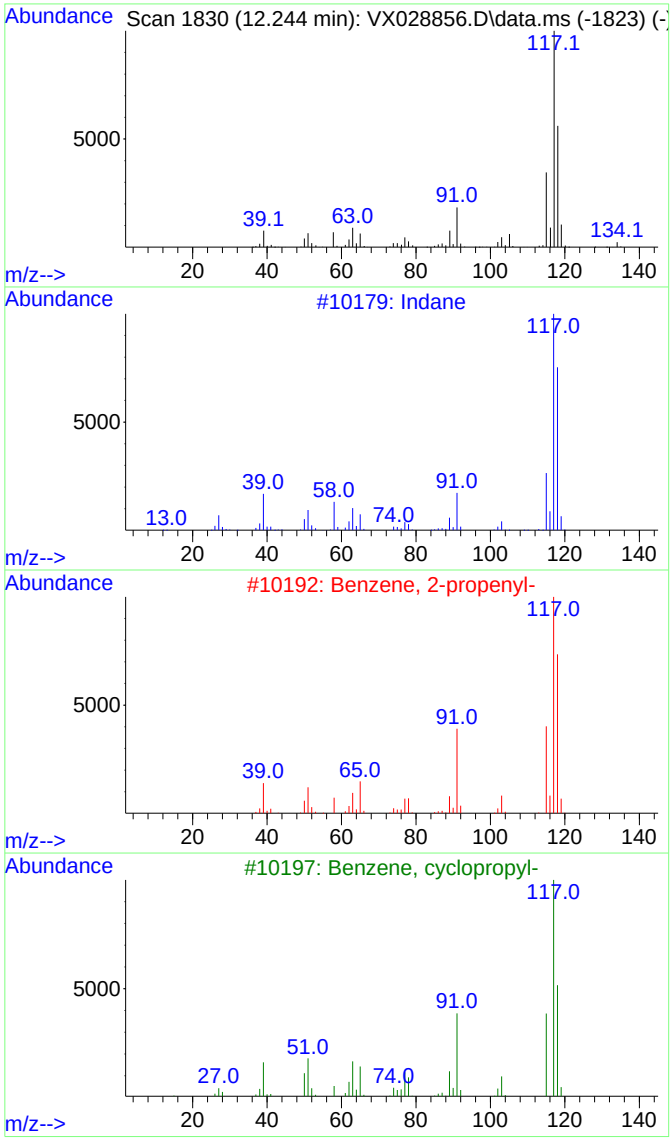
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

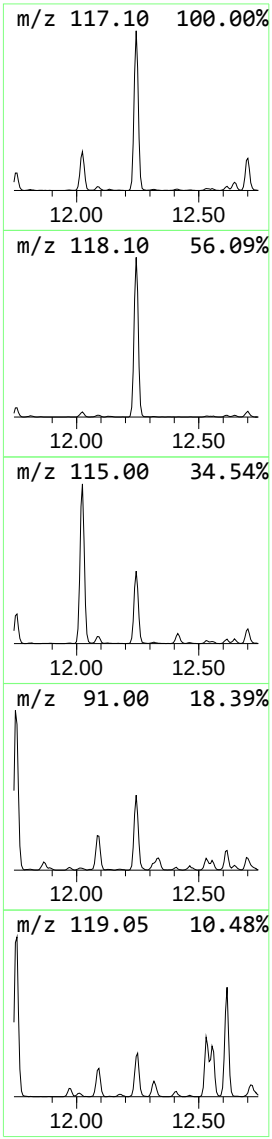
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Indane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	22.41 ug/l	593546	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	87
2	Benzene, 2-propenyl-	118	C9H10	000300-57-2	81
3	Benzene, cyclopropyl-	118	C9H10	000873-49-4	76
4	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	74
5	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	72





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ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-32

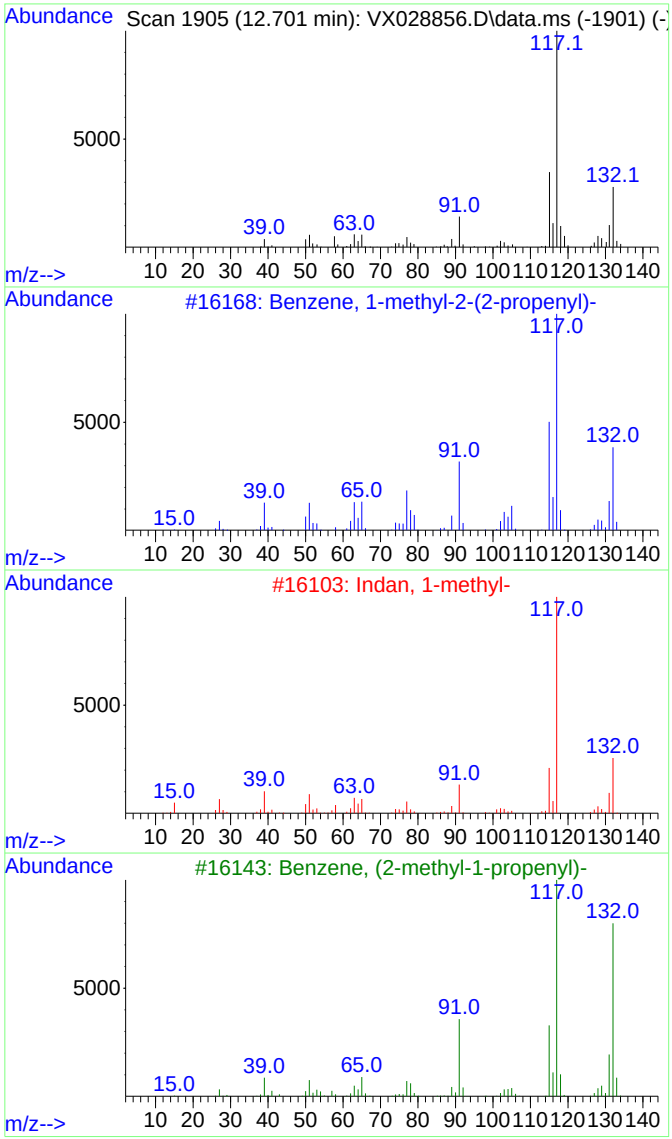
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

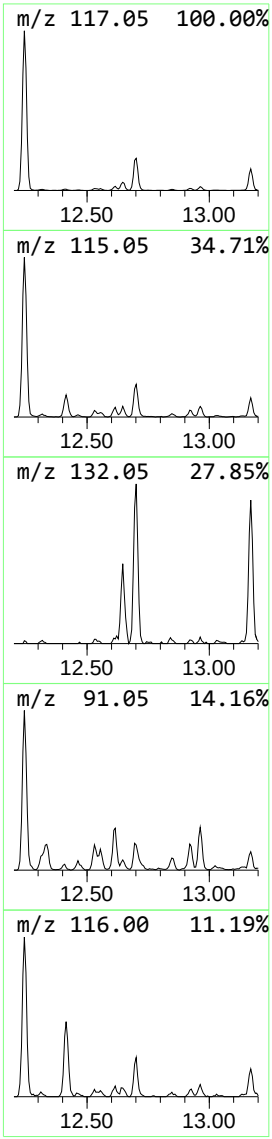
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzene, 1-methyl-2-(2-prop... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.701	5.00 ug/l	132473	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	87
2	Indan, 1-methyl-	132	C10H12	000767-58-8	87
3	Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	86
4	1-Phenyl-1-butene	132	C10H12	000824-90-8	83
5	1H-Indene, 2,3-dihydro-2-methyl-	132	C10H12	000824-63-5	83





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Data File : VX028856.D
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ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-32

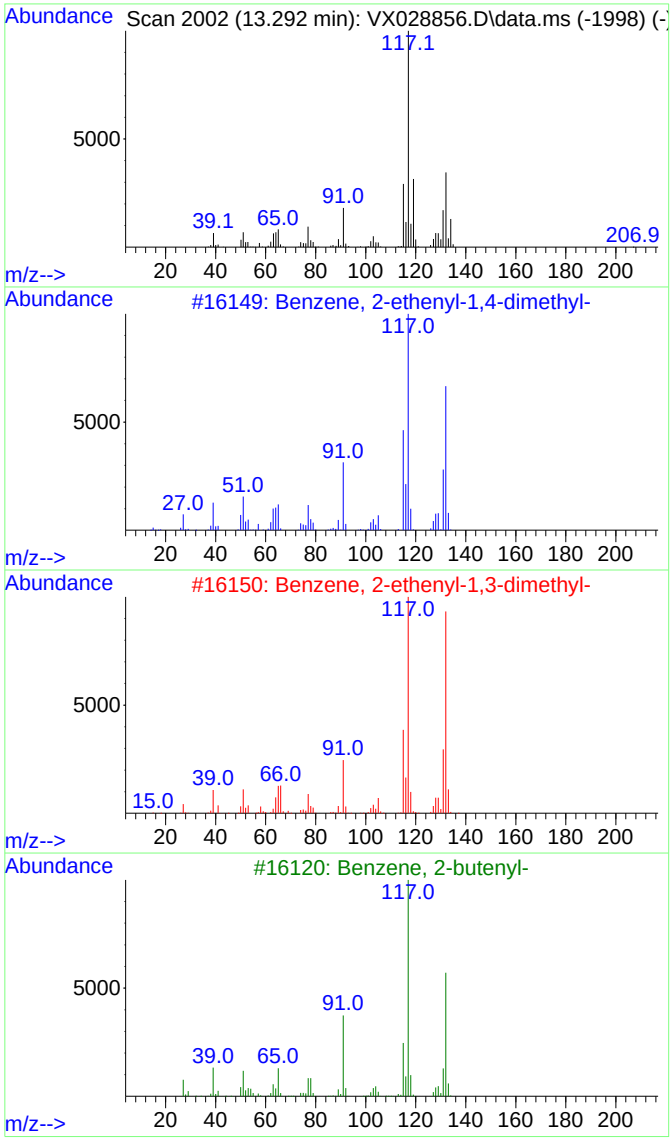
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

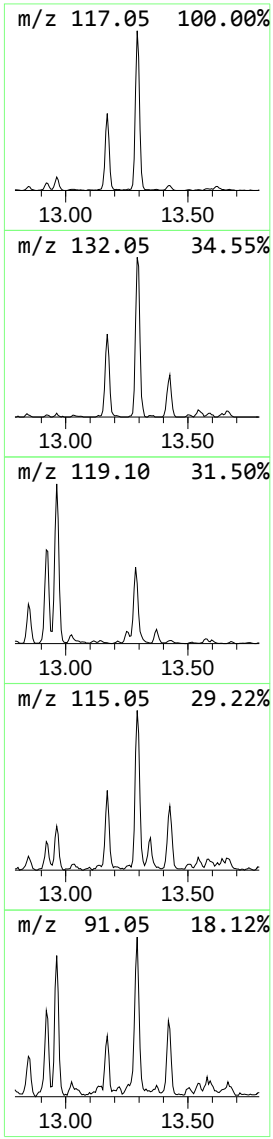
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	7.52 ug/l	199278	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	95
2	Benzene, 2-ethenyl-1,3-dimethyl-	132	C10H12	002039-90-9	90
3	Benzene, 2-butenyl-	132	C10H12	001560-06-1	81
4	1-Phenyl-1-butene	132	C10H12	000824-90-8	81
5	1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	81





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052022\
Data File : VX028856.D
Acq On : 20 May 2022 17:19
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ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
MW-32

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...	1.258	8.2	ug/l	125003	1	5.556	762672	50.0
unknown5.19	11.402	5.2	ug/l	137546	4	12.024	1324440	50.0
Benzene, 1-ethy...	11.616	5.6	ug/l	148678	4	12.024	1324440	50.0
Benzene, 1,2,3-...	12.085	14.9	ug/l	395795	4	12.024	1324440	50.0
Indane	12.244	22.4	ug/l	593546	4	12.024	1324440	50.0
Benzene, 1-meth...	12.701	5.0	ug/l	132473	4	12.024	1324440	50.0
Benzene, 2-ethe...	13.292	7.5	ug/l	199278	4	12.024	1324440	50.0