LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030122\
Data File : VX027248.D
Acq On : 01 Mar 2022 15:06
Operator : JC/MD
Sample : N1688-12
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-29

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\82X022322W.M
Title : SW846 8260

Signal : TIC: VX027248.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.252	22	27	40	rBV2	18152	39105	7.66%	0.803%
2	1.373	42	47	53	rVB	14375	14822	2.90%	0.304%
3	1.751	104	109	117	rVB	21302	29872	5.85%	0.614%
4	1.959	138	143	150	rVB3	7425	12835	2.51%	0.264%
5	2.062	155	160	166	rBV3	5597	9848	1.93%	0.202%
6	2.221	181	186	196	rVB	5913	9755	1.91%	0.200%
7	2.385	209	213	217	rBV	4418	6935	1.36%	0.142%
8	2.538	231	238	251	rBV2	3682	7052	1.38%	0.145%
9	2.757	268	274	282	rBV4	3550	11219	2.20%	0.230%
10	2.873	288	293	301	rVB	9772	19221	3.76%	0.395%
11	2.959	301	307	319	rVB	15325	33101	6.48%	0.680%
12	3.117	323	333	343	rVB3	14597	36065	7.06%	0.741%
13	3.745	428	436	446	rBV5	2014	7234	1.42%	0.149%
14	4.013	472	480	487	rVB3	3695	9240	1.81%	0.190%
15	4.306	520	528	540	rVB3	10289	28792	5.64%	0.591%
16	4.568	565	571	582	rBV	1814	5301	1.04%	0.109%
17	5.391	696	706	715	rBV2	51587	149984	29.36%	3.080%
18	5.476	715	720	725	rVV4	6341	16608	3.25%	0.341%
19	5.562	725	734	749	rVB2	87335	252341	49.40%	5.183%
20	5.964	790	800	805	rBV2	53560	140701	27.54%	2.890%
21	6.043	805	813	828	rVB	192553	510820	100.00%	10.491%
22	6.214	833	841	855	rVB7	3425	15715	3.08%	0.323%
23	6.763	922	931	943	rBV	136763	325389	63.70%	6.683%
24	7.378	1024	1032	1039	rBV3	3478	8602	1.68%	0.177%
25	8.427	1199	1204	1211	rVB2	3434	5886	1.15%	0.121%
26	8.579	1223	1229	1234	rVV	24557	39888	7.81%	0.819%
27	8.653	1234	1241	1248	rVV	297723	458738	89.80%	9.422%
28	8.720	1248	1252	1259	rVB	22420	34531	6.76%	0.709%
29	9.043	1298	1305	1313	rBV3	4414	8792	1.72%	0.181%
30	9.457	1365	1373	1378	rBV4	3899	7105	1.39%	0.146%
31	10.055	1465	1471	1482	rVB	299858	389402	76.23%	7.998%
32	10.195	1489	1494	1501	rBV	224446	286437	56.07%	5.883%
33	10.305	1506	1512	1520	rVB	173119	216836	42.45%	4.453%
34	10.640	1562	1567	1583	rVB	141384	187895	36.78%	3.859%
35	10.963	1615	1620	1625	rBV	12012	14284	2.80%	0.293%
36	11.085	1634	1640	1651	rVB	233921	303467	59.41%	6.233%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030122\
Data File : VX027248.D
Acq On : 01 Mar 2022 15:06
Operator : JC/MD
Sample : N1688-12
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-29

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\82X022322W.M
Title : SW846 8260

37	11.305	1671	1676	1682	rBV	23896	28247	5.53%	0.580%
38	11.402	1682	1692	1696	rVV	36232	60410	11.83%	1.241%
39	11.451	1696	1700	1709	rVB	9396	12452	2.44%	0.256%
40	11.616	1722	1727	1735	rVB	51032	64303	12.59%	1.321%
41	11.756	1744	1750	1758	rBV	196294	240852	47.15%	4.947%
42	12.024	1789	1794	1800	rBV	325806	393796	77.09%	8.088%
43	12.085	1800	1804	1811	rVB	69734	88303	17.29%	1.814%
44	12.243	1822	1830	1838	rBV	69004	95803	18.75%	1.968%
45	12.317	1838	1842	1848	rVB4	6206	9798	1.92%	0.201%
46	12.414	1854	1858	1863	rBV3	6346	8153	1.60%	0.167%
47	12.530	1873	1877	1880	rBV	6700	9930	1.94%	0.204%
48	12.615	1887	1891	1894	rBV	12623	13708	2.68%	0.282%
49	12.701	1900	1905	1913	rVB2	12347	16800	3.29%	0.345%
50	12.853	1925	1930	1934	rVV2	4185	5713	1.12%	0.117%
51	12.920	1937	1941	1945	rBV	7822	9562	1.87%	0.196%
52	12.963	1945	1948	1954	rVB	10421	12302	2.41%	0.253%
53	13.170	1978	1982	1986	rVB	8488	10187	1.99%	0.209%
54	13.292	1993	2002	2007	rBV2	23851	32604	6.38%	0.670%
55	13.426	2020	2024	2028	rVB2	6854	9090	1.78%	0.187%
56	13.774	2074	2081	2088	rBV	52624	71500	14.00%	1.468%
57	14.639	2220	2223	2226	rVB	6816	7314	1.43%	0.150%
58	14.780	2239	2246	2251	rBV2	10174	14382	2.82%	0.295%

Sum of corrected areas: 4869027

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Acq On : 01 Mar 2022 15:06
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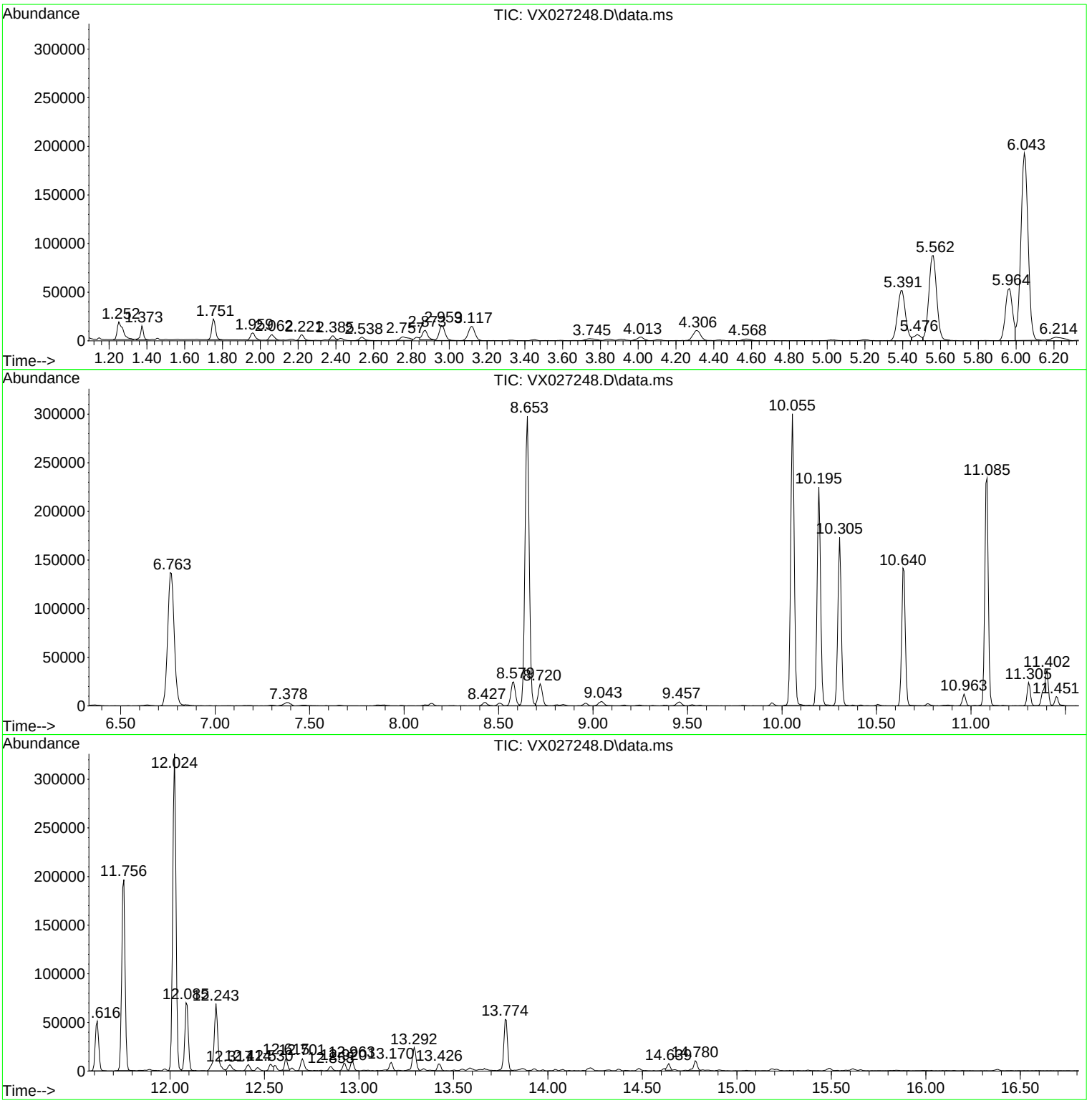
Sample : N1688-12
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-29

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022322W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030122\
Data File : VX027248.D
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Operator : JC/MD
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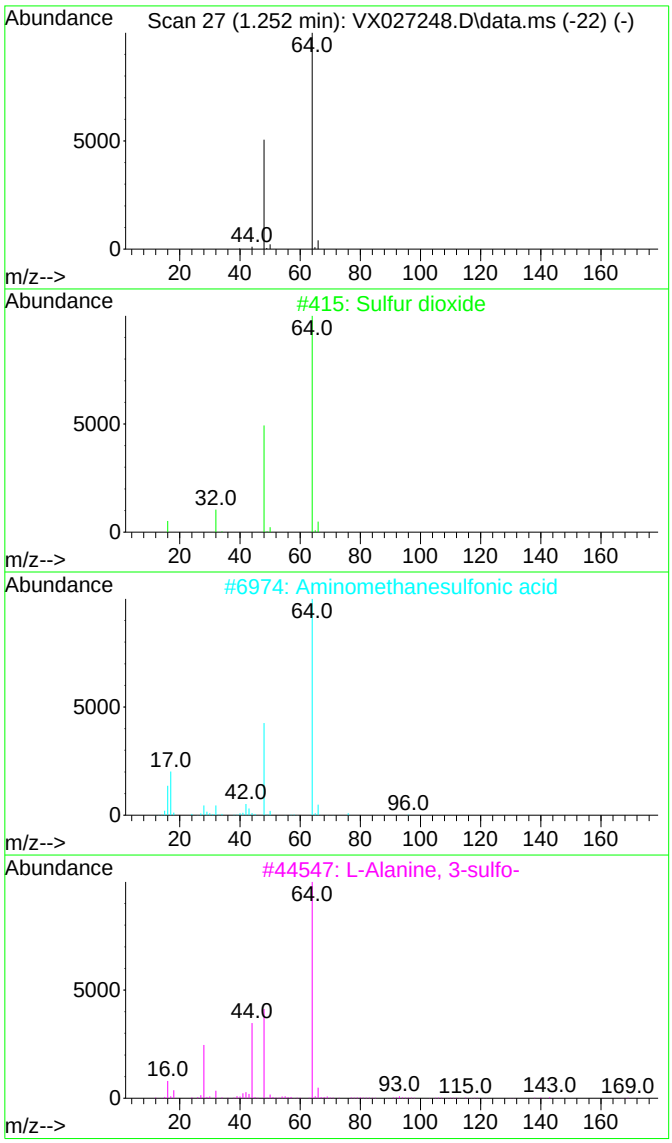
Quant Title : SW846 8260

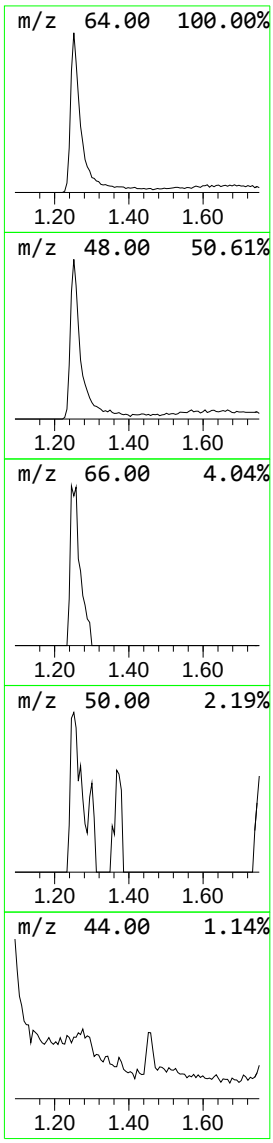
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Sulfur dioxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.252	7.75 ug/l	39105	Pentafluorobenzene	5.562

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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Data File : VX027248.D
Acq On : 01 Mar 2022 15:06
Operator : JC/MD
Sample : N1688-12
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-29

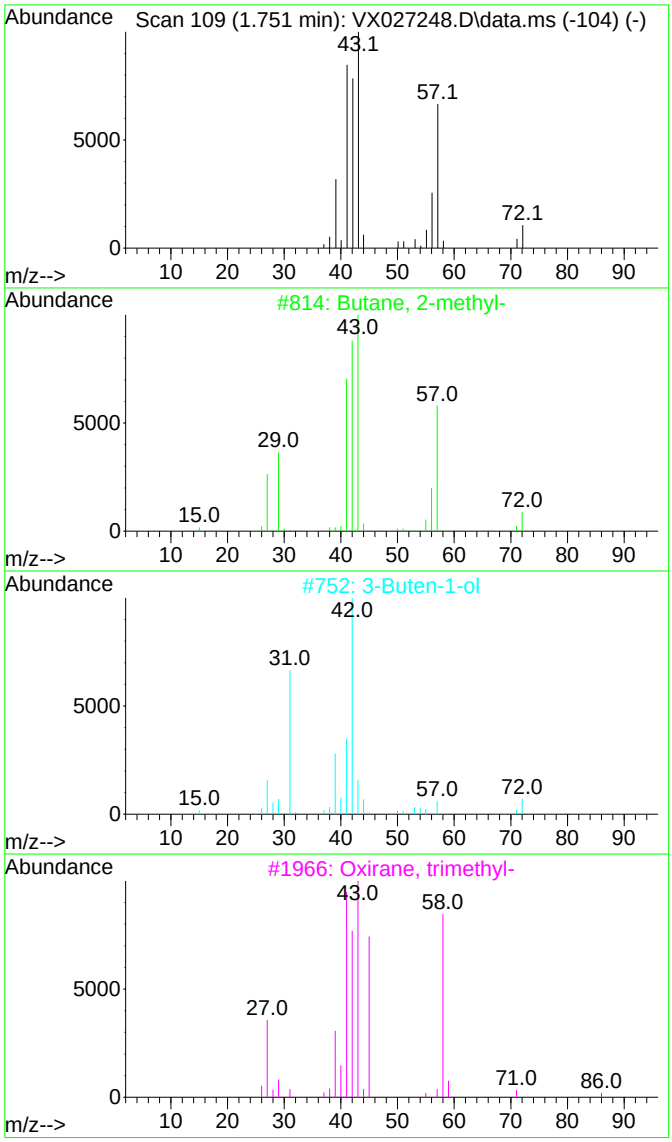
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022322W.M
Quant Title : SW846 8260

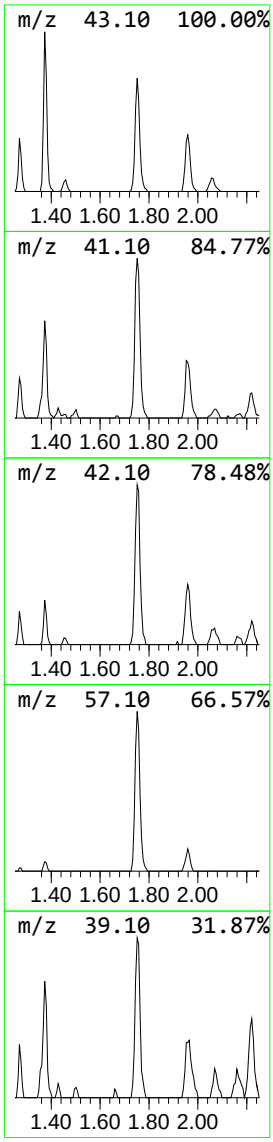
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.751	5.92 ug/l	29872	Pentafluorobenzene	5.562

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	47
3	Oxirane, trimethyl-	86	C5H10O	005076-19-7	42
4	Pentane	72	C5H12	000109-66-0	38
5	1,3-Dimethyldiaziridine	72	C3H8N2	026177-36-6	28





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Data File : VX027248.D
Acq On : 01 Mar 2022 15:06
Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-29

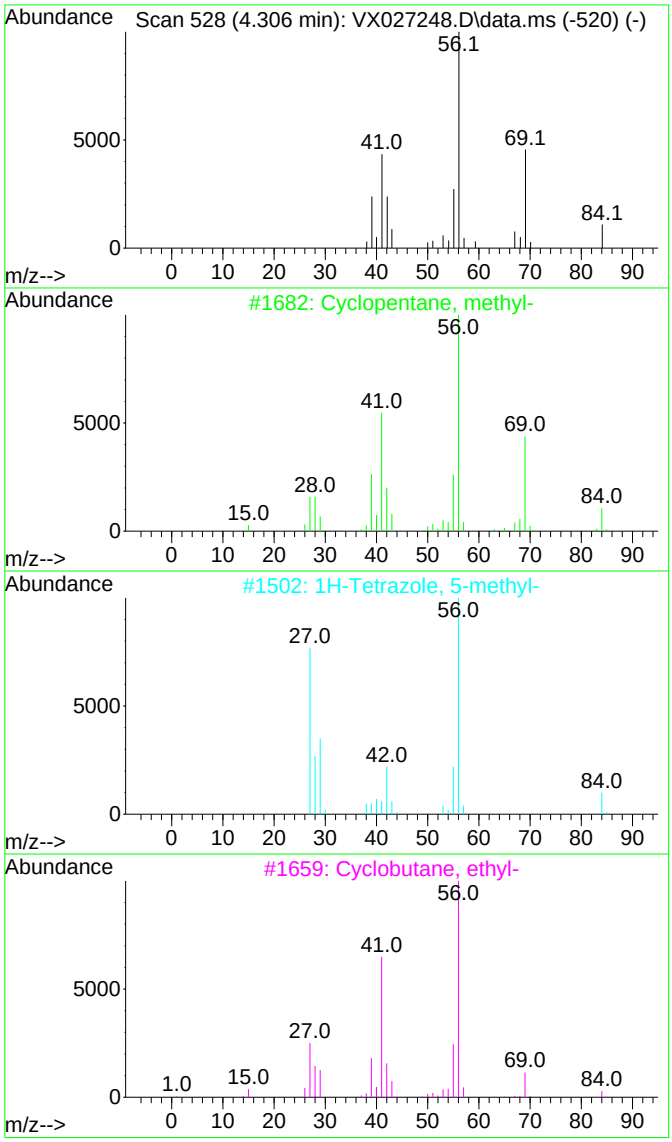
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022322W.M
Quant Title : SW846 8260

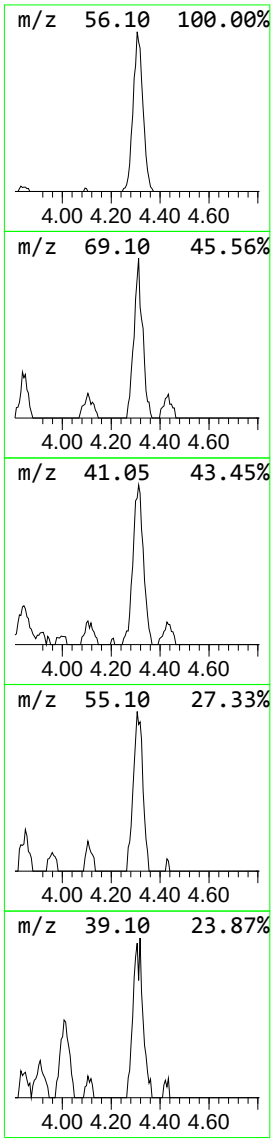
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Cyclopentane, methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.306	5.70 ug/l	28792	Pentafluorobenzene	5.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	80
3	Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
4	2H-Pyran-2,6(3H)-dione, dihydro-...	142	C7H10O3	004160-82-1	45
5	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	43





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030122\
Data File : VX027248.D
Acq On : 01 Mar 2022 15:06
Operator : JC/MD
Sample : N1688-12
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-29

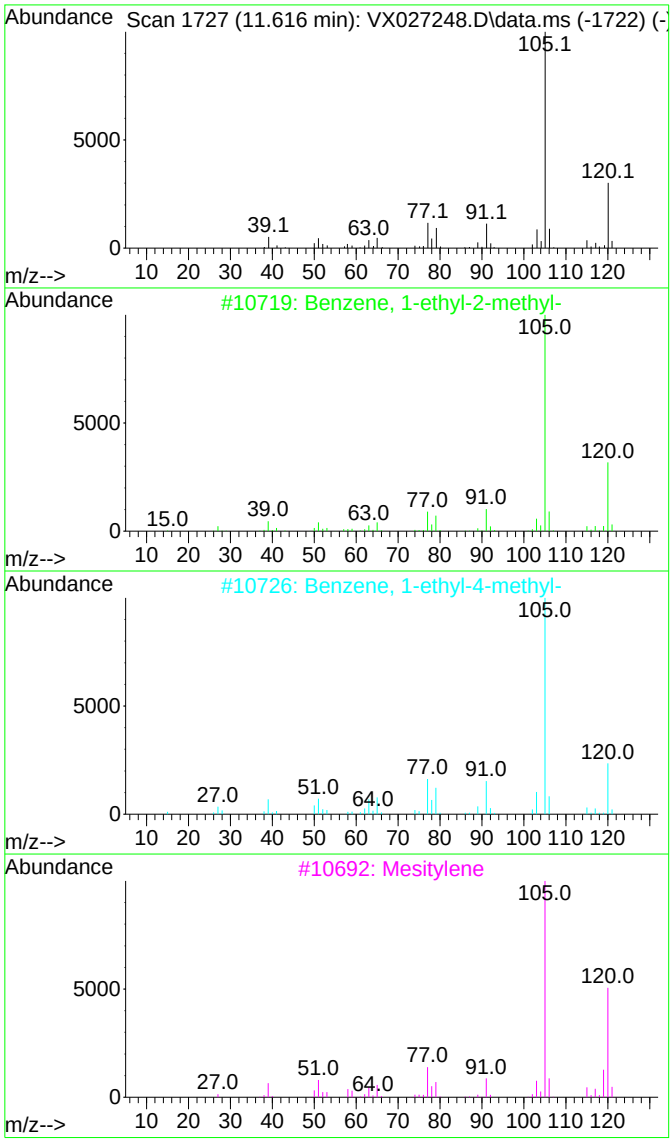
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022322W.M
Quant Title : SW846 8260

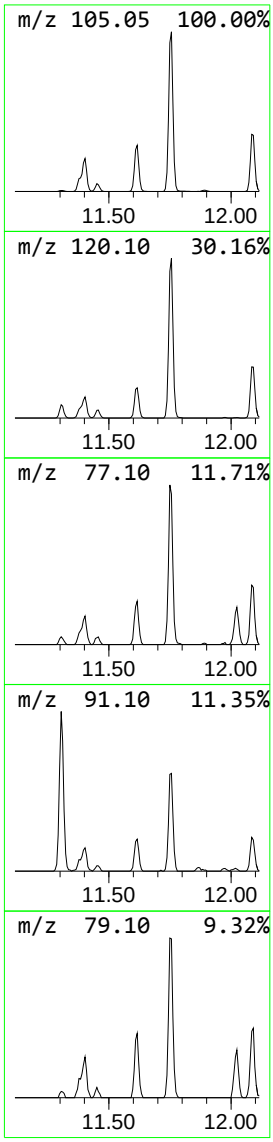
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.616	8.16 ug/l	64303	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	94
2	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	94
3	Mesitylene	120	C9H12	000108-67-8	91
4	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
5	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91





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Data File : VX027248.D
Acq On : 01 Mar 2022 15:06
Operator : JC/MD
Sample : N1688-12
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-29

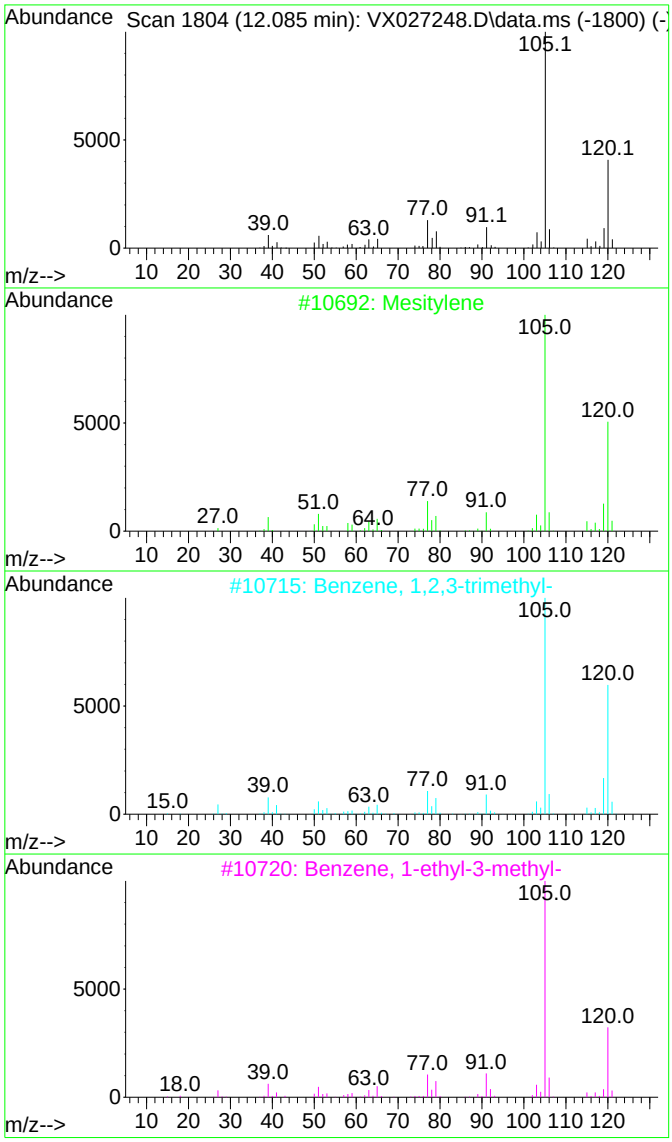
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022322W.M
Quant Title : SW846 8260

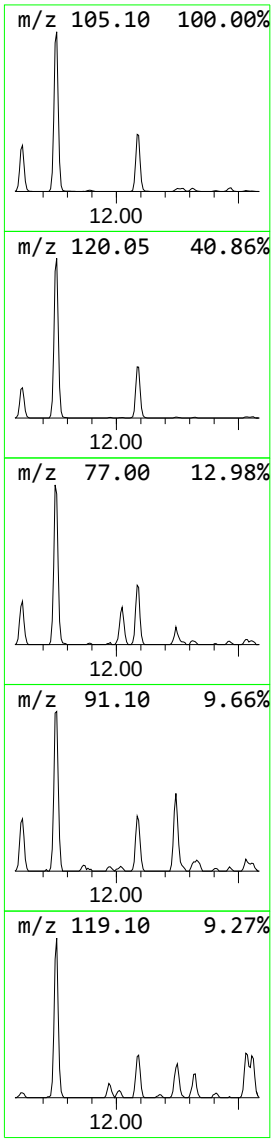
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.085	11.21 ug/l	88303	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-2-methyl-	120	C9H12	000611-14-3	90





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Instrument :
MSVOA_X
ClientSampleId :
MW-29

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022322W.M
Quant Title : SW846 8260

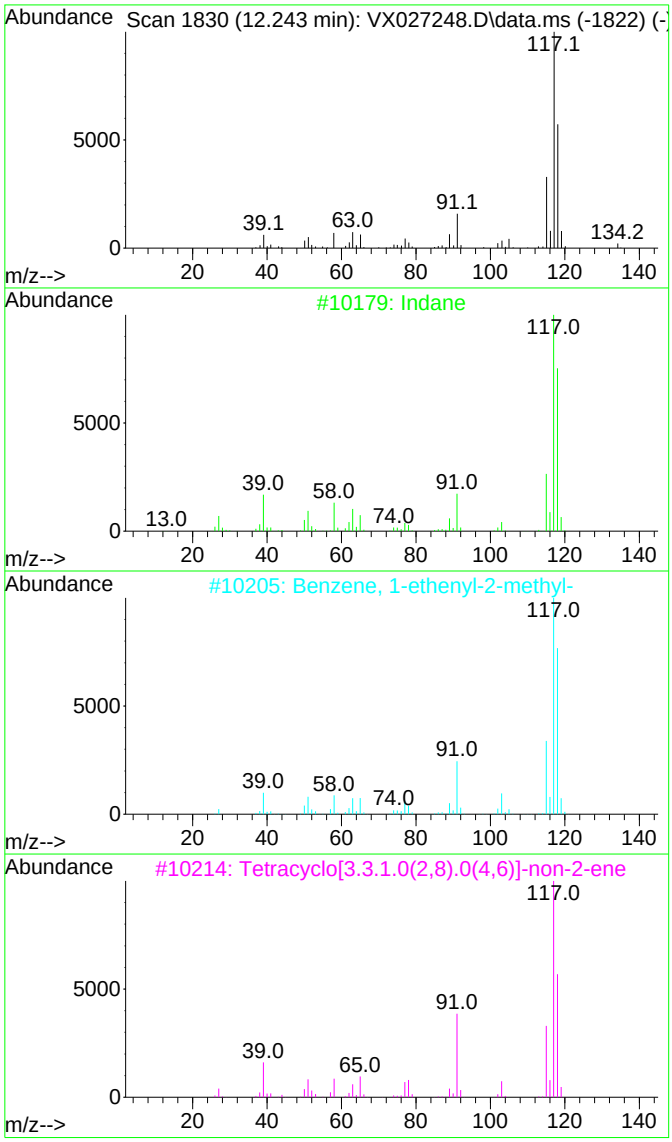
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

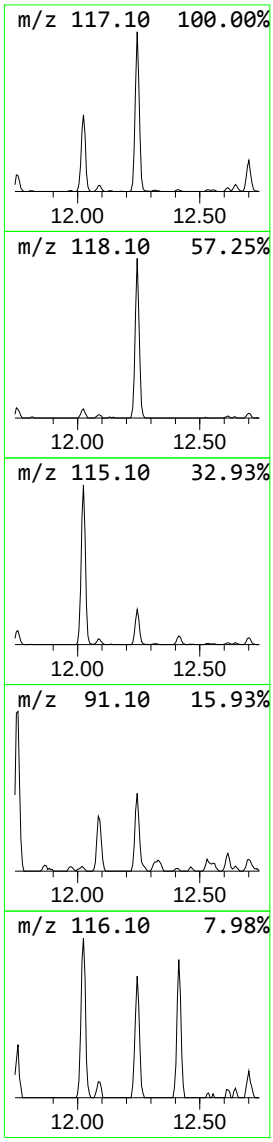
****

Peak Number 6 Indane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.243	12.16 ug/l	95803	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	91
2	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	81
3	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	80
4	Benzene, 1,1'-(1-ethenyl-1,3-pro...	222	C17H18	061141-97-7	78
5	Benzene, 1-propenyl-	118	C9H10	000637-50-3	74





Tentatively Identified Compound (LSC) summary

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Data File : VX027248.D
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ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-29

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022322W.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	1.252	7.8	ug/l	39105	1	5.562	252341	50.0
Butane, 2-methyl-	1.751	5.9	ug/l	29872	1	5.562	252341	50.0
Cyclopentane, m...	4.306	5.7	ug/l	28792	1	5.562	252341	50.0
Benzene, 1-ethy...	11.616	8.2	ug/l	64303	4	12.024	393796	50.0
Benzene, 1,2,3-...	12.085	11.2	ug/l	88303	4	12.024	393796	50.0
Indane	12.243	12.2	ug/l	95803	4	12.024	393796	50.0