LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112522\
Data File : VX033071.D
Acq On : 25 Nov 2022 16:28
Operator : JC/MD
Sample : N5747-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 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\82X112222W.M
Title : SW846 8260

Signal : TIC: VX033071.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.246	22	26	41	rBV	79202	168627	11.86%	1.657%
2	1.374	41	47	52	rVB	47402	57905	4.07%	0.569%
3	1.752	104	109	116	rVB	66125	85981	6.05%	0.845%
4	1.965	138	144	154	rVV3	39961	80861	5.69%	0.794%
5	2.069	156	161	168	rVV	20060	30534	2.15%	0.300%
6	2.166	169	177	181	rVV2	16654	27029	1.90%	0.266%
7	2.215	181	185	194	rVB	57953	87071	6.13%	0.855%
8	2.751	262	273	281	rBV	28106	61248	4.31%	0.602%
9	2.867	287	292	304	rVB2	28853	64970	4.57%	0.638%
10	2.989	304	312	324	rVV3	6584	23823	1.68%	0.234%
11	3.111	324	332	346	rVB2	24226	58959	4.15%	0.579%
12	3.733	425	434	445	rVB5	9096	24662	1.74%	0.242%
13	3.843	445	452	457	rBV	6295	14297	1.01%	0.140%
14	4.105	485	495	506	rVB3	6964	17302	1.22%	0.170%
15	4.306	518	528	540	rBV2	21735	61684	4.34%	0.606%
16	5.196	663	674	684	rVB2	11566	33812	2.38%	0.332%
17	5.391	694	706	714	rBV	62168	182218	12.82%	1.790%
18	5.477	714	720	724	rVV2	14536	40035	2.82%	0.393%
19	5.550	724	732	750	rVB	136597	391396	27.54%	3.845%
20	5.958	787	799	804	rBV	67670	171898	12.09%	1.689%
21	6.037	804	812	828	rVB	534588	1421309	100.00%	13.964%
22	6.202	828	839	845	rBV2	8546	23378	1.64%	0.230%
23	6.763	920	931	941	rBV	207347	495973	34.90%	4.873%
24	7.379	1022	1032	1044	rVB5	6637	15856	1.12%	0.156%
25	8.647	1234	1240	1247	rBV	314489	494471	34.79%	4.858%
26	8.720	1247	1252	1261	rVB	160921	242302	17.05%	2.381%
27	9.458	1366	1373	1378	rBV3	9665	16155	1.14%	0.159%
28	10.055	1465	1471	1484	rVB	425806	572924	40.31%	5.629%
29	10.195	1488	1494	1505	rBV	840642	1092454	76.86%	10.733%
30	10.305	1505	1512	1521	rVB	801611	1110792	78.15%	10.913%
31	10.640	1562	1567	1575	rBV	199744	251572	17.70%	2.472%
32	10.963	1615	1620	1625	rBV	34001	41850	2.94%	0.411%
33	11.079	1634	1639	1650	rBV	272939	352242	24.78%	3.461%
34	11.305	1671	1676	1682	rBV	60631	73746	5.19%	0.725%
35	11.378	1683	1688	1690	rVV	69388	97338	6.85%	0.956%
36	11.396	1690	1691	1696	rVV	84151	85399	6.01%	0.839%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112522\
Data File : VX033071.D
Acq On : 25 Nov 2022 16:28
Operator : JC/MD
Sample : N5747-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 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\82X112222W.M
Title : SW846 8260

37	11.451	1696	1700	1709	rVB	52240	61978	4.36%	0.609%
38	11.610	1721	1726	1734	rBV	83615	108831	7.66%	1.069%
39	11.750	1744	1749	1756	rBV	437780	521102	36.66%	5.120%
40	12.024	1788	1794	1800	rBV	440293	555381	39.08%	5.456%
41	12.085	1800	1804	1810	rVB	154201	193351	13.60%	1.900%
42	12.244	1824	1830	1838	rBV	170372	219126	15.42%	2.153%
43	12.317	1838	1842	1849	rVB3	10604	16247	1.14%	0.160%
44	12.414	1853	1858	1862	rBV	16505	21030	1.48%	0.207%
45	12.530	1873	1877	1879	rBV	13297	15465	1.09%	0.152%
46	12.609	1886	1890	1894	rBV	18708	24325	1.71%	0.239%
47	12.701	1900	1905	1912	rBV2	22160	30693	2.16%	0.302%
48	12.920	1936	1941	1945	rBV	12467	15439	1.09%	0.152%
49	12.963	1945	1948	1953	rVB	17285	19724	1.39%	0.194%
50	13.170	1977	1982	1992	rVB	17175	21610	1.52%	0.212%
51	13.292	1992	2002	2007	rBV3	41063	56882	4.00%	0.559%
52	13.426	2019	2024	2030	rVB	13387	17710	1.25%	0.174%
53	13.774	2076	2081	2088	rBV	129866	167364	11.78%	1.644%
54	14.640	2218	2223	2232	rVB	14917	18699	1.32%	0.184%
55	14.780	2241	2246	2252	rBV	17696	21398	1.51%	0.210%

Sum of corrected areas: 10178428

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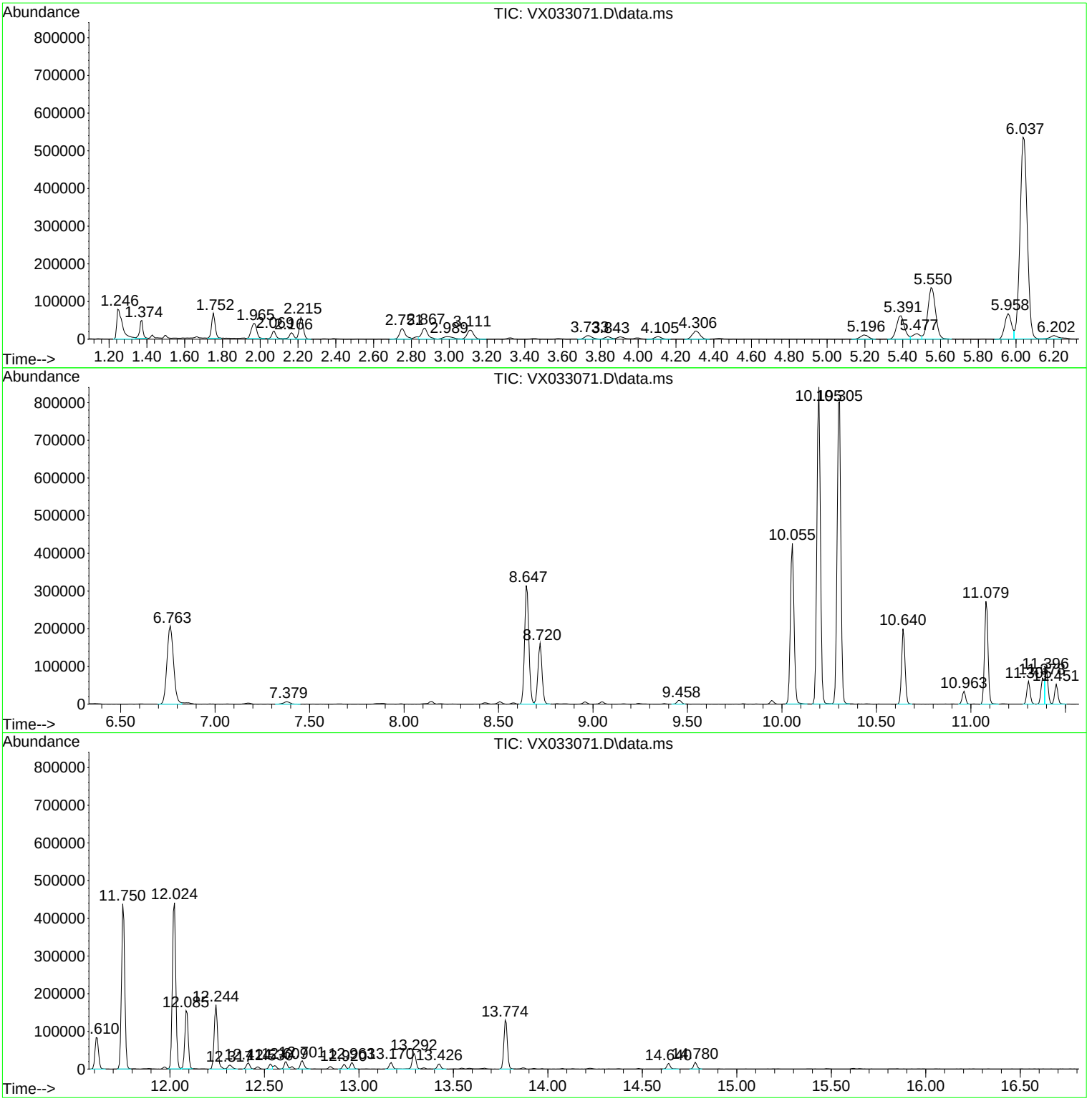
Sample : N5747-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-29

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112522\
Data File : VX033071.D
Acq On : 25 Nov 2022 16:28
Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-29

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

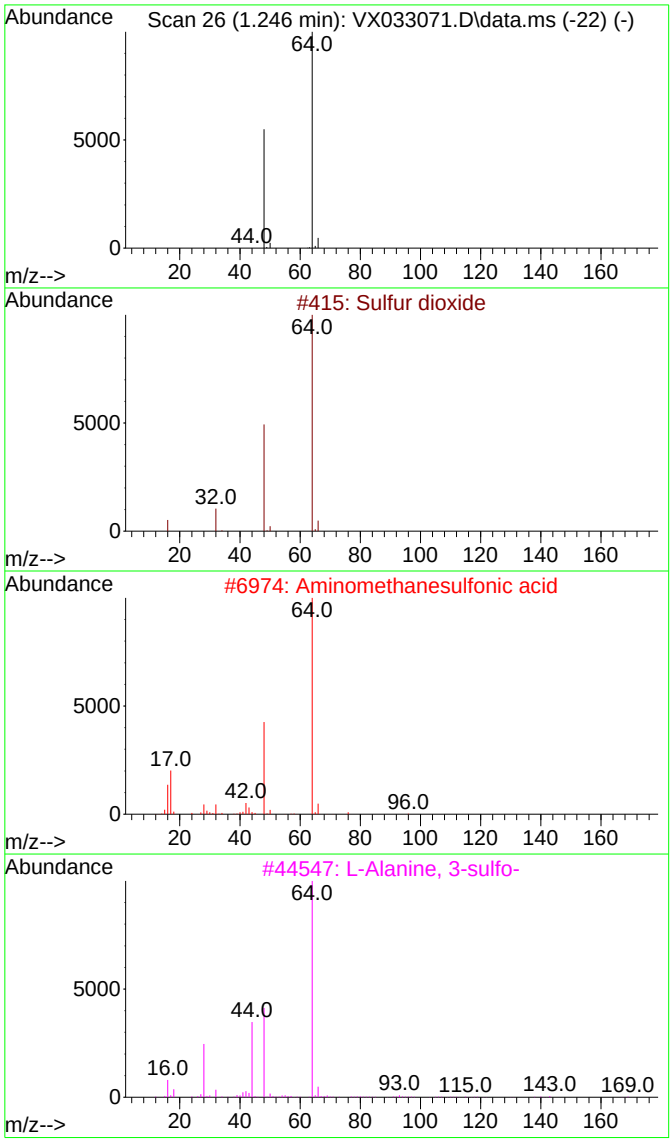
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

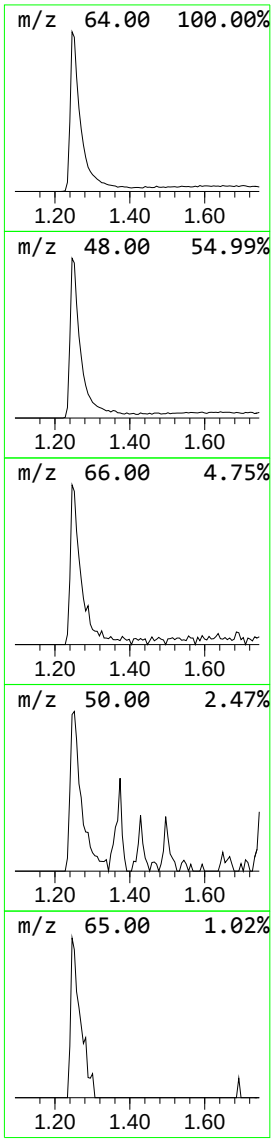
****

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.246	21.54 ug/l	168627	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	Ethene, 1,2-difluoro-	64	C2H2F2	001691-13-0	3





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112522\
Data File : VX033071.D
Acq On : 25 Nov 2022 16:28
Operator : JC/MD
Sample : N5747-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-29

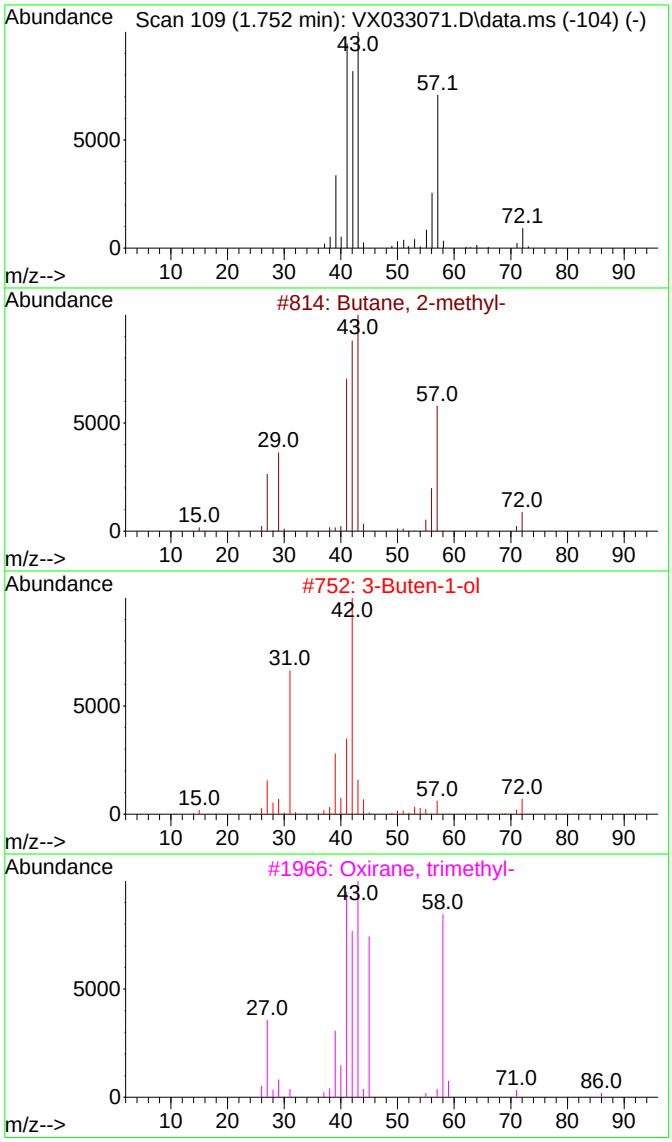
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

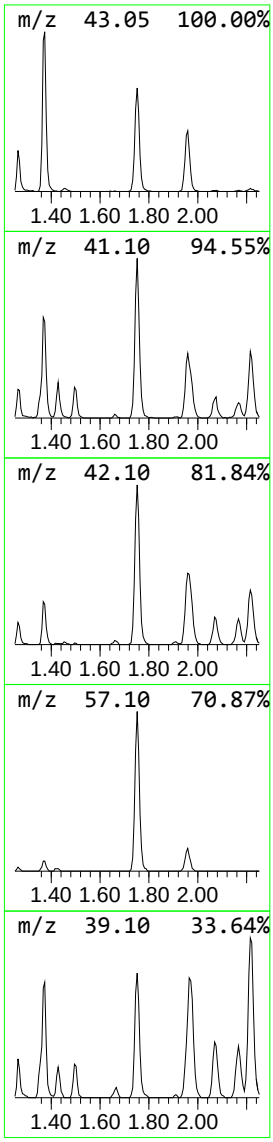
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.752	10.98 ug/l	85981	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	42
4	2(3H)-Furanone, dihydro-4-methyl-	100	C5H8O2	001679-49-8	33
5	Pentane	72	C5H12	000109-66-0	33





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112522\
Data File : VX033071.D
Acq On : 25 Nov 2022 16:28
Operator : JC/MD
Sample : N5747-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-29

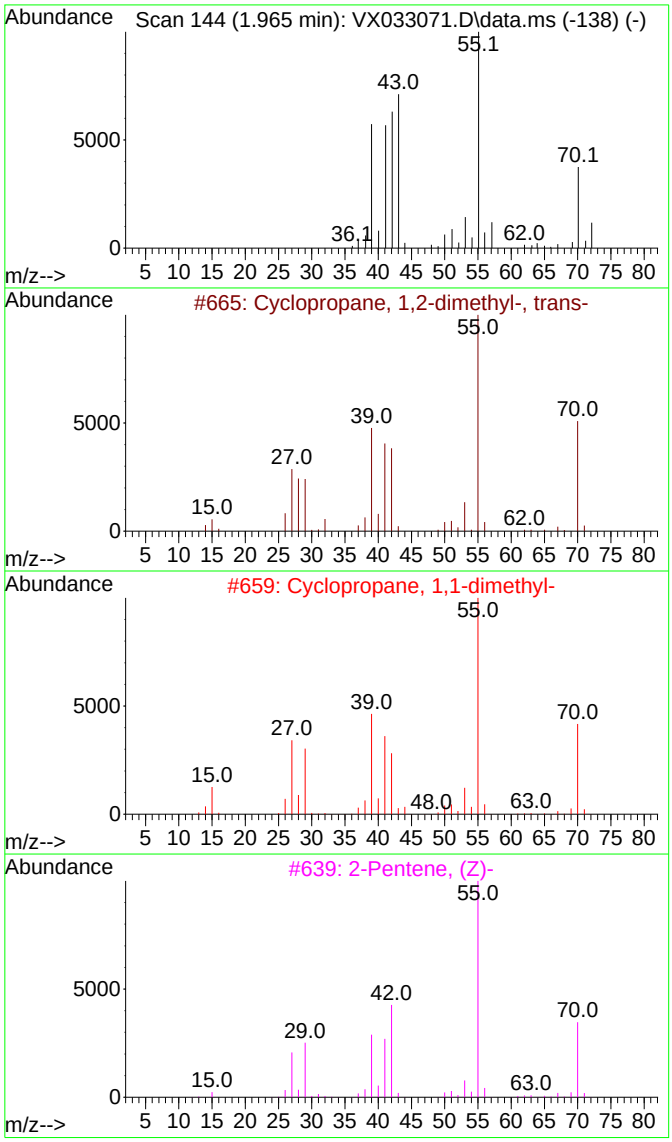
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

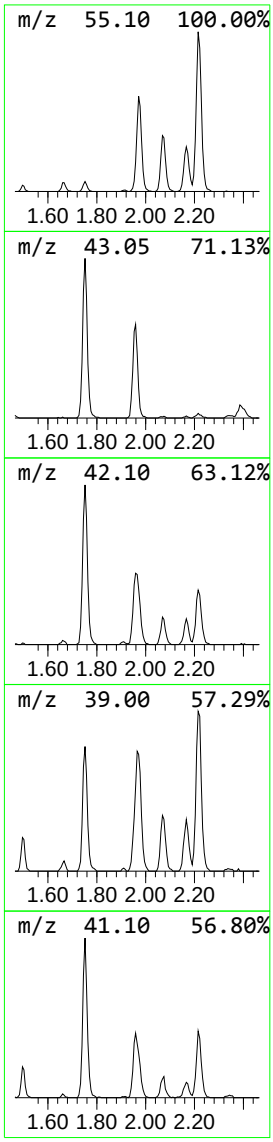
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Cyclopropane, 1,2-dimethyl-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.965	10.33 ug/l	80861	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	62
2	Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	62
3	2-Pentene, (Z)-	70	C5H10	000627-20-3	52
4	1-Butene, 3-methyl-	70	C5H10	000563-45-1	49
5	2-Pentene, (E)-	70	C5H10	000646-04-8	49





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112522\
Data File : VX033071.D
Acq On : 25 Nov 2022 16:28
Operator : JC/MD
Sample : N5747-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-29

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

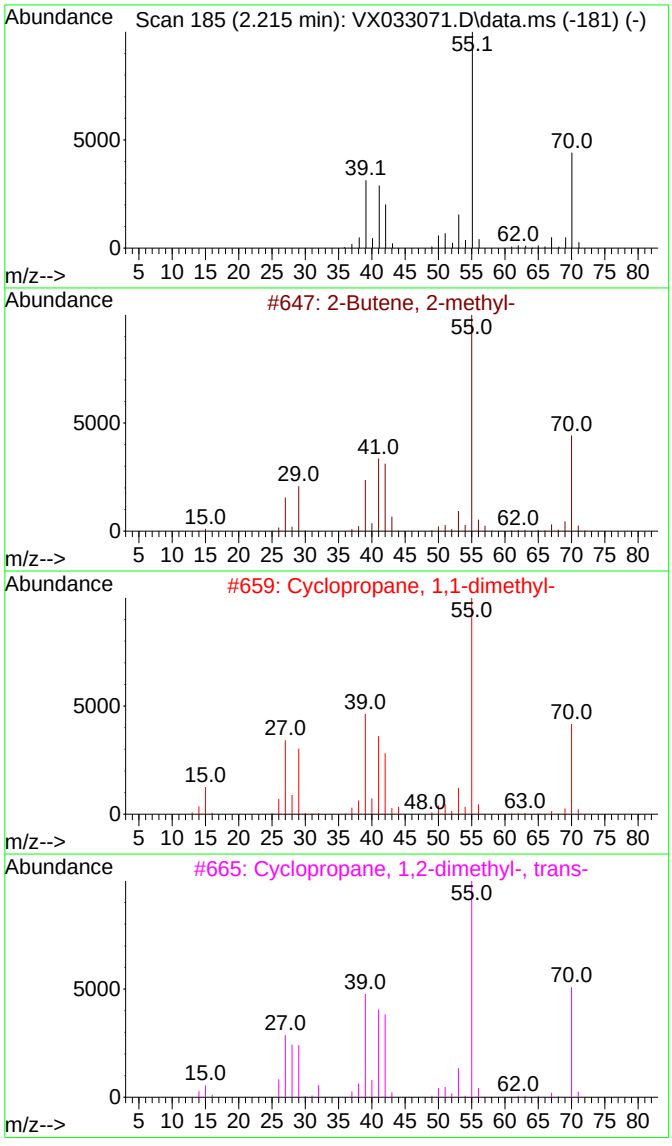
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

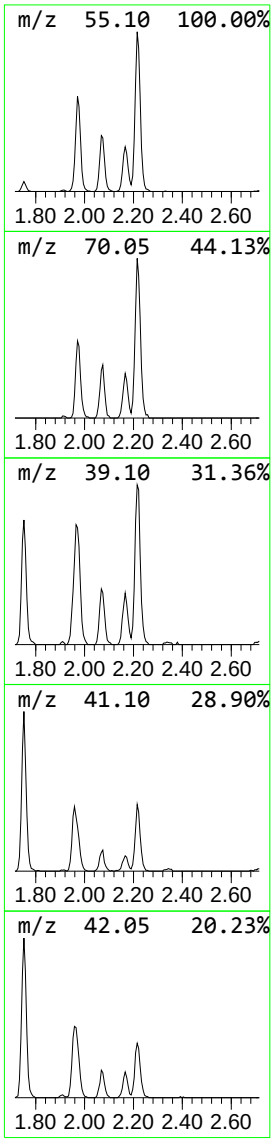
****

Peak Number 4 2-Butene, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.215	11.12 ug/l	87071	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butene, 2-methyl-	70	C5H10	000513-35-9	90
2	Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	80
3	Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	72
4	2-Pentene, (E)-	70	C5H10	000646-04-8	72
5	2-Pentene, (Z)-	70	C5H10	000627-20-3	72





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112522\
Data File : VX033071.D
Acq On : 25 Nov 2022 16:28
Operator : JC/MD
Sample : N5747-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-29

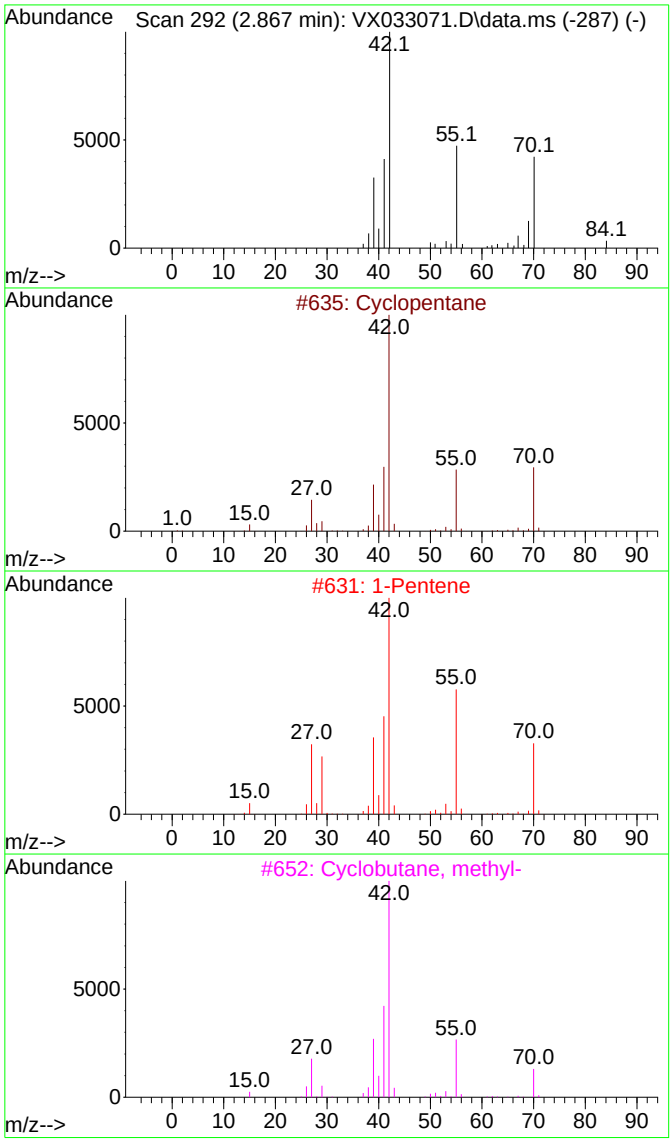
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

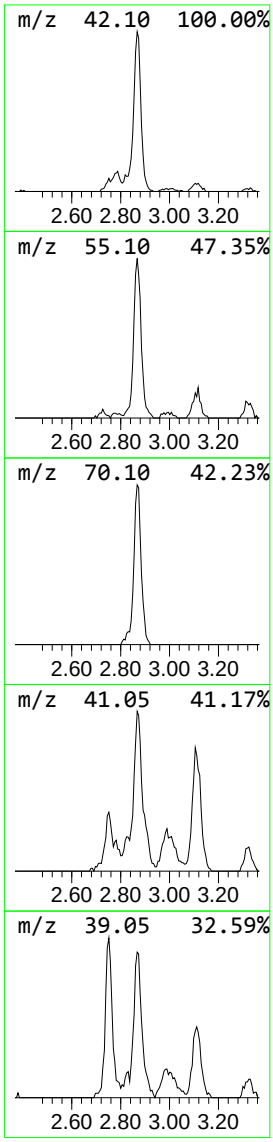
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Cyclopentane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.867	8.30 ug/l	64970	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	50
3	Cyclobutane, methyl-	70	C5H10	000598-61-8	50
4	Cyclopropane, ethyl-	70	C5H10	001191-96-4	50
5	Cyclobutanone	70	C4H6O	001191-95-3	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112522\
Data File : VX033071.D
Acq On : 25 Nov 2022 16:28
Operator : JC/MD
Sample : N5747-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-29

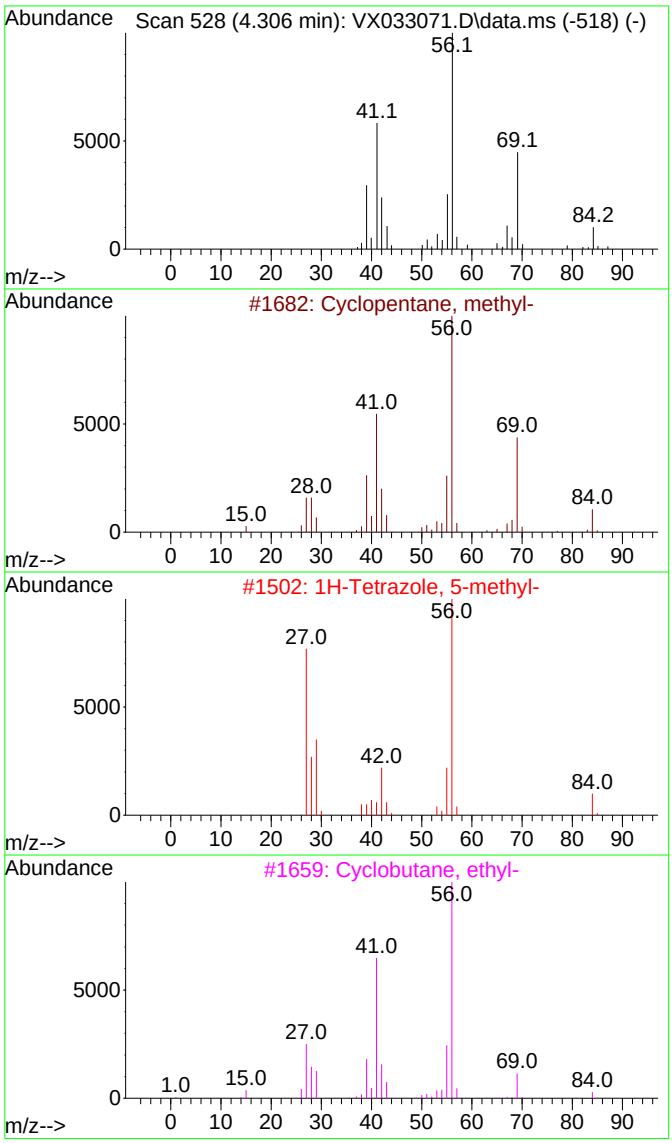
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

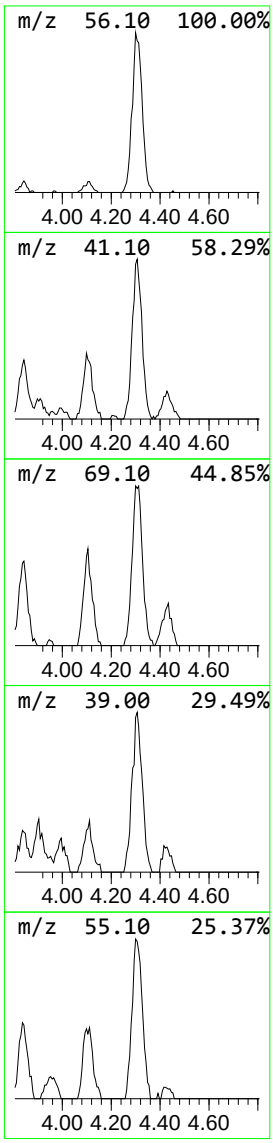
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Cyclopentane, methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.306	7.88 ug/l	61684	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	87
2	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	64
3	Cyclobutane, ethyl-	84	C6H12	004806-61-5	59
4	Cyclohexane	84	C6H12	000110-82-7	56
5	Cyclobutane	56	C4H8	000287-23-0	43





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112522\
Data File : VX033071.D
Acq On : 25 Nov 2022 16:28
Operator : JC/MD
Sample : N5747-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-29

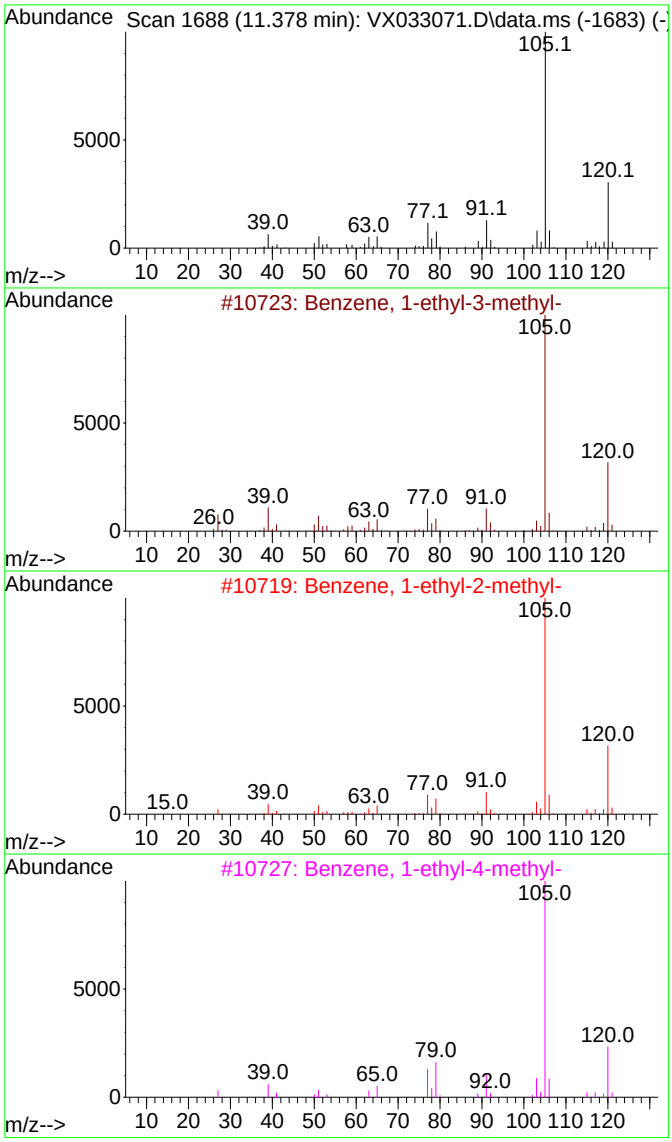
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

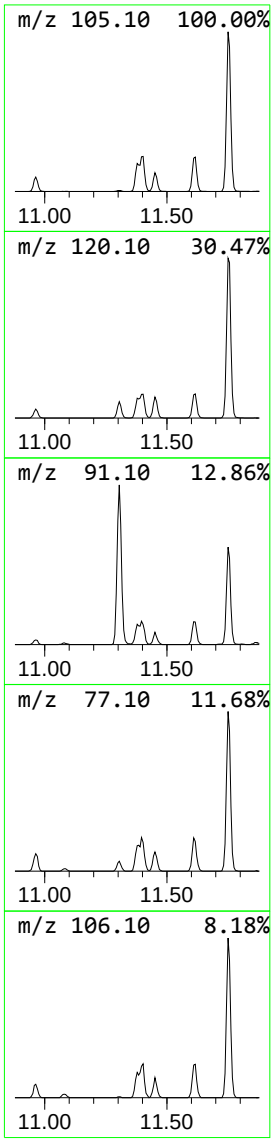
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, 1-ethyl-3-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.378	8.76 ug/l	97338	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	94
2	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
3	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5	Mesitylene	120	C9H12	000108-67-8	90





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112522\
Data File : VX033071.D
Acq On : 25 Nov 2022 16:28
Operator : JC/MD
Sample : N5747-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-29

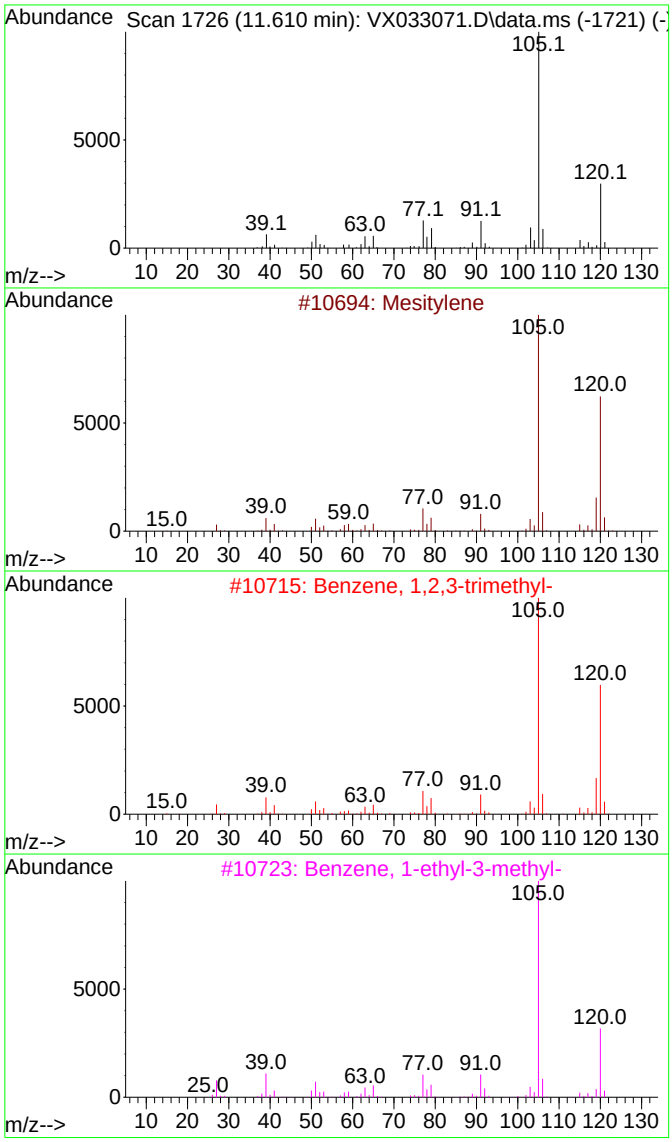
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

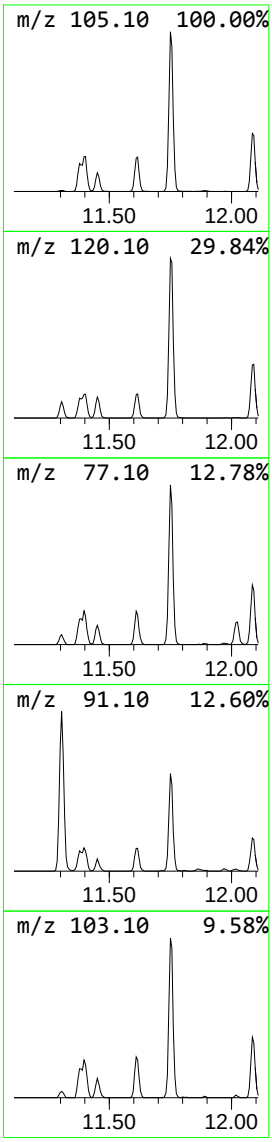
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, 1-ethyl-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.610	9.80 ug/l	108831	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Mesitylene	120	C9H12	000108-67-8	91
2	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
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	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112522\
Data File : VX033071.D
Acq On : 25 Nov 2022 16:28
Operator : JC/MD
Sample : N5747-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-29

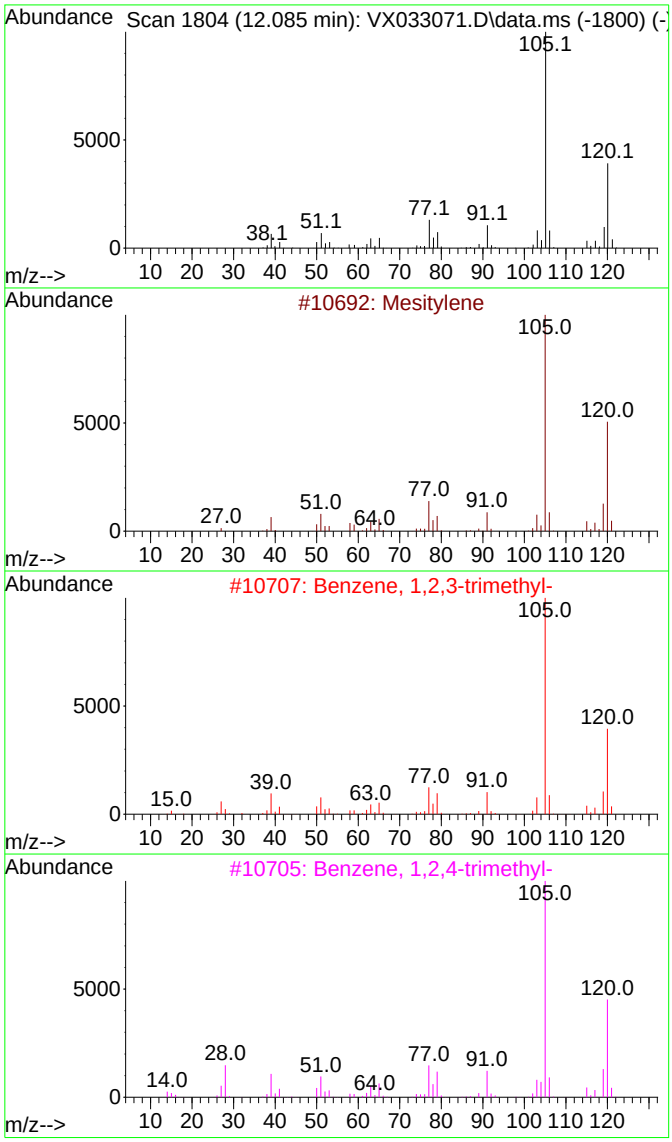
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

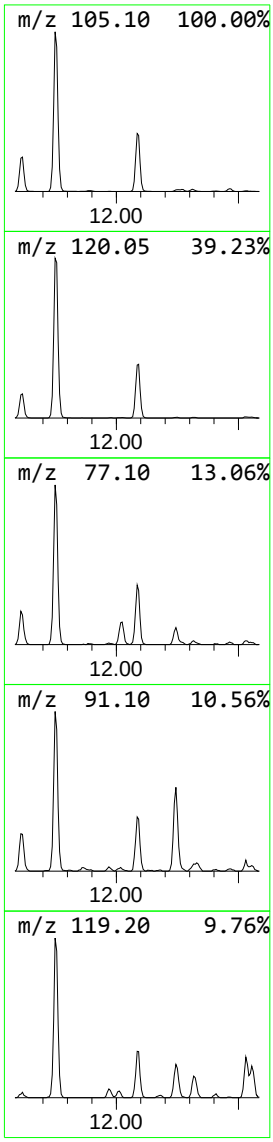
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.085	17.41 ug/l	193351	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	97
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	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112522\
Data File : VX033071.D
Acq On : 25 Nov 2022 16:28
Operator : JC/MD
Sample : N5747-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-29

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

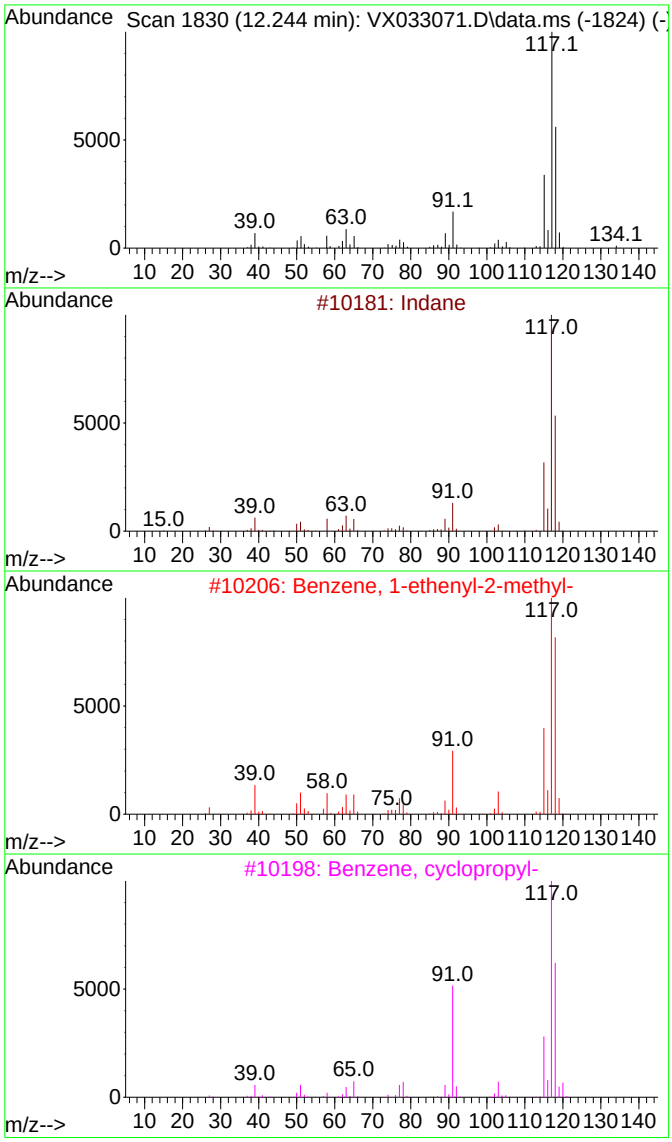
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

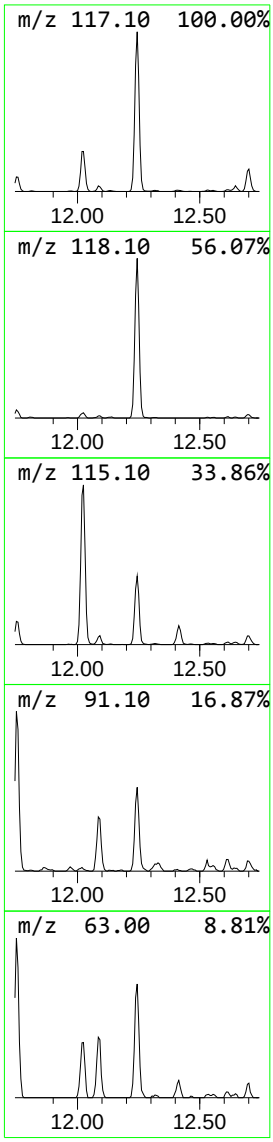
****

Peak Number 10 Indane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	19.73 ug/l	219126	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	93
2	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	87
3	Benzene, cyclopropyl-	118	C9H10	000873-49-4	83
4	Deltacyclene	118	C9H10	007785-10-6	72
5	(Z)-1-Phenylpropene	118	C9H10	000766-90-5	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112522\
Data File : VX033071.D
Acq On : 25 Nov 2022 16:28
Operator : JC/MD
Sample : N5747-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-29

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.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	1.246	21.5	ug/l	168627	1	5.556	391396	50.0
Butane, 2-methyl-	1.752	11.0	ug/l	85981	1	5.556	391396	50.0
Cyclopropane, 1...	1.965	10.3	ug/l	80861	1	5.556	391396	50.0
2-Butene, 2-met...	2.215	11.1	ug/l	87071	1	5.556	391396	50.0
Cyclopentane	2.867	8.3	ug/l	64970	1	5.556	391396	50.0
Cyclopentane, m...	4.306	7.9	ug/l	61684	1	5.556	391396	50.0
Benzene, 1-ethy...	11.378	8.8	ug/l	97338	4	12.024	555381	50.0
Benzene, 1-ethy...	11.610	9.8	ug/l	108831	4	12.024	555381	50.0
Benzene, 1,2,3-...	12.085	17.4	ug/l	193351	4	12.024	555381	50.0
Indane	12.244	19.7	ug/l	219126	4	12.024	555381	50.0