LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061121\
Data File : VX022670.D
Acq On : 11 Jun 2021 16:19
Operator : JC/MD
Sample : M2688-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-2

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\82X061021W.M
Title : SW846 8260

Signal : TIC: VX022670.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.374	41	47	53	rBV	415586	420554	1.73%	0.354%
2	1.746	103	108	123	rVB	983970	1401961	5.76%	1.180%
3	1.953	138	142	155	rVB2	585461	926358	3.81%	0.780%
4	2.069	155	161	169	rBV	515173	708555	2.91%	0.596%
5	2.166	171	177	181	rVV	293181	437826	1.80%	0.369%
6	2.215	181	185	195	rVB	572274	852405	3.50%	0.717%
7	2.752	258	273	281	rBV2	285311	868958	3.57%	0.731%
8	2.831	281	286	289	rVV	350725	750270	3.08%	0.632%
9	2.867	289	292	307	rVB2	385041	853324	3.51%	0.718%
10	3.105	320	331	346	rVB	269290	597380	2.46%	0.503%
11	3.447	377	387	401	rVB	206234	465129	1.91%	0.392%
12	4.312	519	529	542	rVB	719307	2057986	8.46%	1.732%
13	5.483	711	721	731	rBV2	622134	1989490	8.18%	1.675%
14	5.629	741	745	763	rVB2	91023	275372	1.13%	0.232%
15	5.836	767	779	791	rBV5	96133	307911	1.27%	0.259%
16	6.050	804	814	825	rVB	2249631	5930374	24.38%	4.992%
17	6.257	840	848	858	rVV5	246610	824796	3.39%	0.694%
18	6.367	858	866	877	rVB2	88006	249093	1.02%	0.210%
19	6.769	924	932	939	rBV	128320	316034	1.30%	0.266%
20	7.385	1019	1033	1044	rBV3	342789	897097	3.69%	0.755%
21	8.110	1143	1152	1156	rBV	231246	484775	1.99%	0.408%
22	8.653	1236	1241	1246	rVB	243910	393137	1.62%	0.331%
23	8.738	1246	1255	1261	rBV	14194654	24329130	100.00%	20.479%
24	10.055	1461	1471	1476	rBV	255542	390073	1.60%	0.328%
25	10.201	1489	1495	1501	rBV	3703500	4916741	20.21%	4.139%
26	10.311	1506	1513	1527	rVB	11442356	15839968	65.11%	13.333%
27	10.646	1562	1568	1578	rBV	5062951	6609214	27.17%	5.563%
28	10.964	1614	1620	1627	rBV	629328	811001	3.33%	0.683%
29	11.085	1635	1640	1644	rBV	206040	263860	1.08%	0.222%
30	11.311	1668	1677	1683	rBV	1319989	1706391	7.01%	1.436%
31	11.384	1683	1689	1690	rVV	1863542	2148092	8.83%	1.808%
32	11.402	1690	1692	1696	rVV	2393265	2748688	11.30%	2.314%
33	11.457	1696	1701	1712	rVB	2367805	2818609	11.59%	2.373%
34	11.616	1721	1727	1735	rBV	3129653	3839266	15.78%	3.232%
35	11.762	1745	1751	1756	rBV	9689932	12075979	49.64%	10.165%
36	12.024	1789	1794	1799	rVB2	306046	430578	1.77%	0.362%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061121\
Data File : VX022670.D
Acq On : 11 Jun 2021 16:19
Operator : JC/MD
Sample : M2688-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-2

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\82X061021W.M
Title : SW846 8260

37	12.091	1799	1805	1810	rBV	3122756	3749604	15.41%	3.156%
38	12.250	1825	1831	1838	rBV3	1589580	2408075	9.90%	2.027%
39	12.323	1838	1843	1850	rVB3	861280	1316965	5.41%	1.109%
40	12.463	1862	1866	1872	rVB	365778	457144	1.88%	0.385%
41	12.536	1872	1878	1880	rBV	744502	977244	4.02%	0.823%
42	12.561	1880	1882	1886	rVB	572102	569457	2.34%	0.479%
43	12.616	1886	1891	1895	rBV	1198983	1398346	5.75%	1.177%
44	12.701	1901	1905	1916	rBV2	327071	551299	2.27%	0.464%
45	12.853	1925	1930	1935	rVB	319700	386786	1.59%	0.326%
46	12.927	1935	1942	1945	rBV	652031	802984	3.30%	0.676%
47	12.969	1945	1949	1954	rVB	860076	1062172	4.37%	0.894%
48	13.170	1975	1982	1987	rBV	401843	477600	1.96%	0.402%
49	13.292	1998	2002	2008	rVB2	979515	1328721	5.46%	1.118%
50	13.780	2076	2082	2087	rBV	1275827	1549346	6.37%	1.304%
51	14.640	2215	2223	2228	rBV	363330	425197	1.75%	0.358%
52	14.780	2241	2246	2256	rVB	315841	405544	1.67%	0.341%

Sum of corrected areas: 118802859

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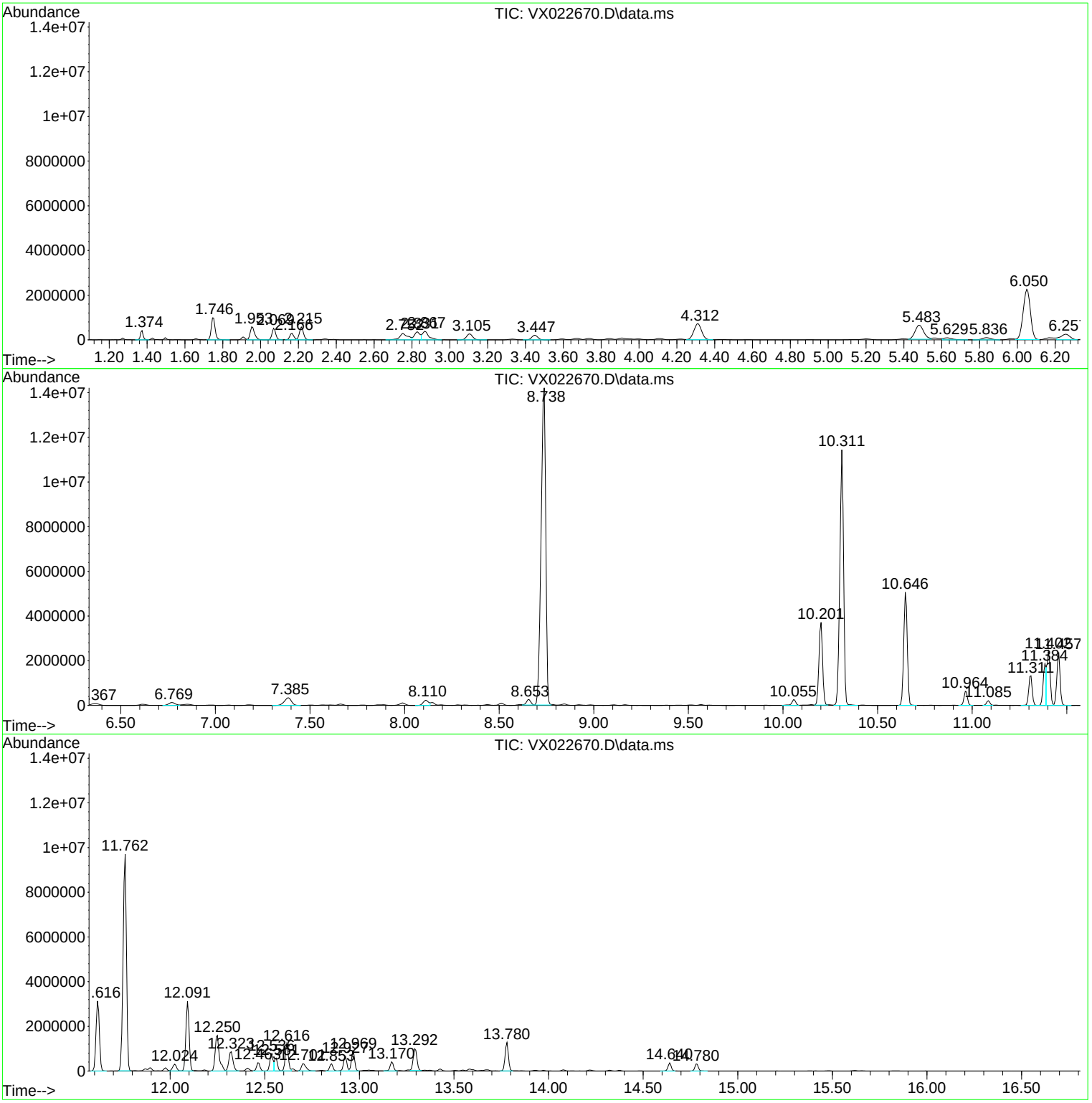
Data File : VX022670.D
Acq On : 11 Jun 2021 16:19
Operator : JC/MD
Sample : M2688-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061021W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061121\
Data File : VX022670.D
Acq On : 11 Jun 2021 16:19
Operator : JC/MD
Sample : M2688-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-2

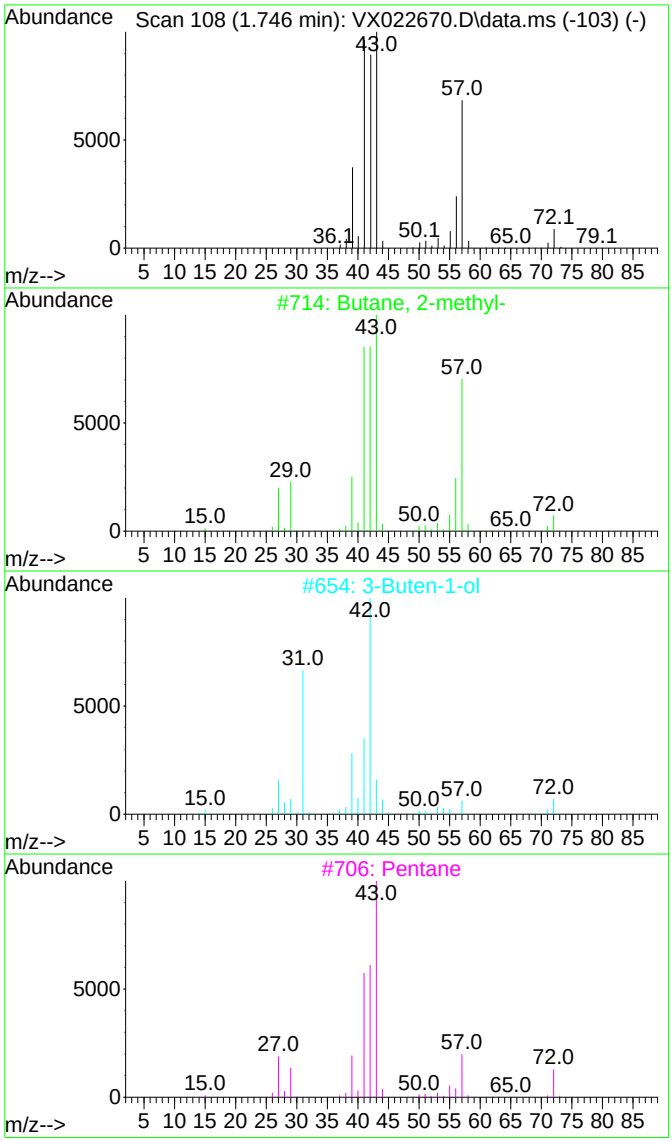
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061021W.M
Quant Title : SW846 8260

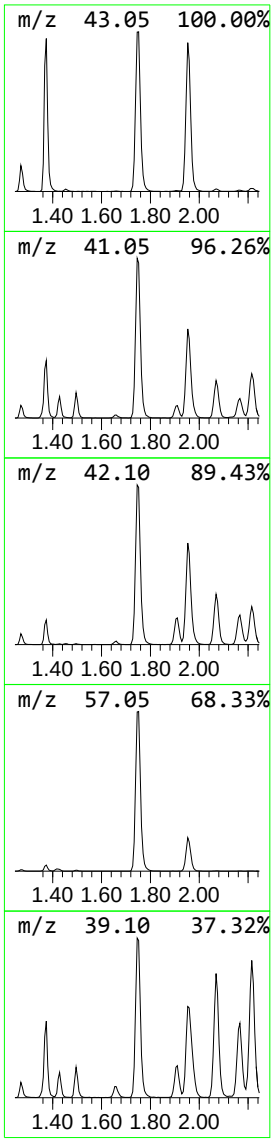
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Butane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.746	254.56 ug/l	1401960	Pentafluorobenzene	5.568

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	91
2	3-Buten-1-ol	72	C4H8O	000627-27-0	47
3	Pentane	72	C5H12	000109-66-0	36
4	1-Butene	56	C4H8	000106-98-9	9
5	Azetidine	57	C3H7N	000503-29-7	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061121\
Data File : VX022670.D
Acq On : 11 Jun 2021 16:19
Operator : JC/MD
Sample : M2688-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061021W.M
Quant Title : SW846 8260

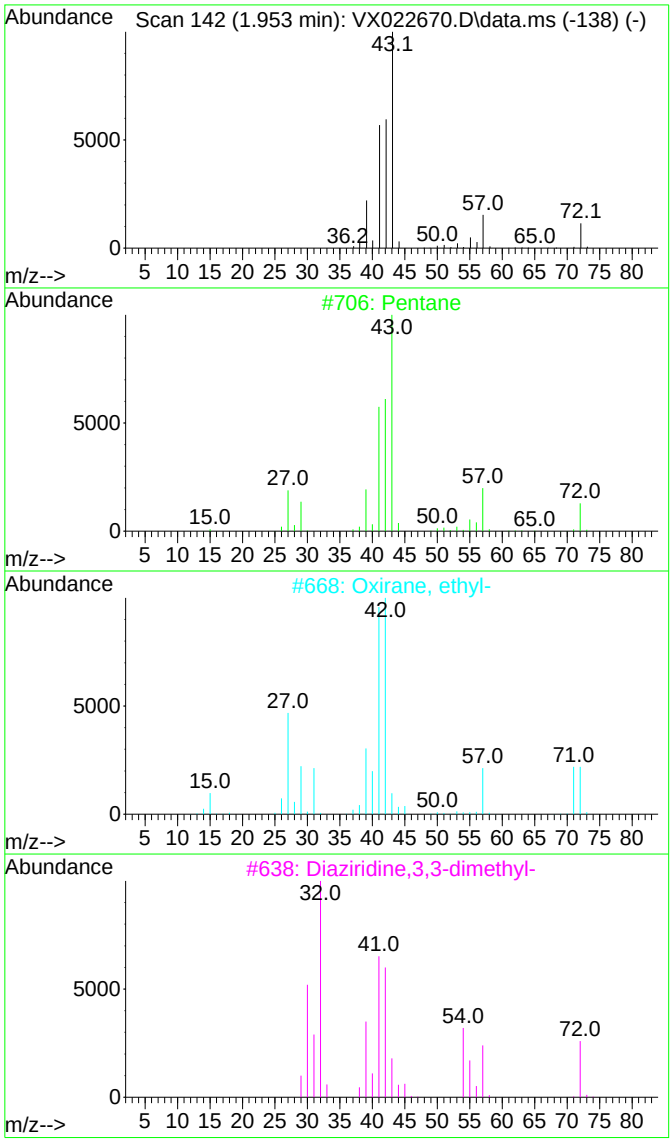
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

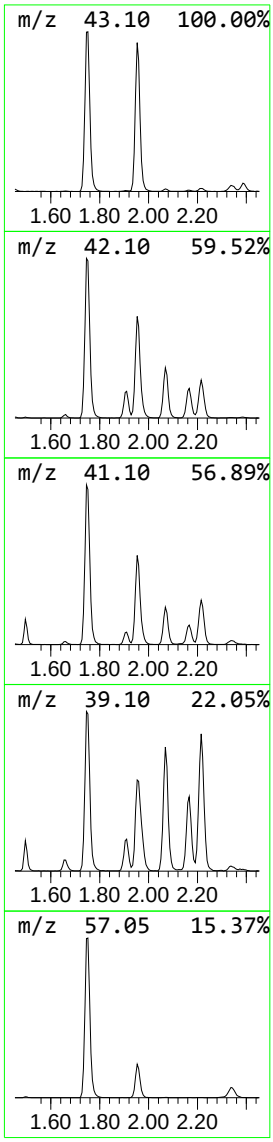
****

Peak Number 2 Pentane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.953	168.20 ug/l	926358	Pentafluorobenzene	5.568

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane	72	C5H12	000109-66-0	91
2	Oxirane, ethyl-	72	C4H8O	000106-88-7	40
3	Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	35
4	Butane, 2-methyl-	72	C5H12	000078-78-4	10
5	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061121\
Data File : VX022670.D
Acq On : 11 Jun 2021 16:19
Operator : JC/MD
Sample : M2688-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-2

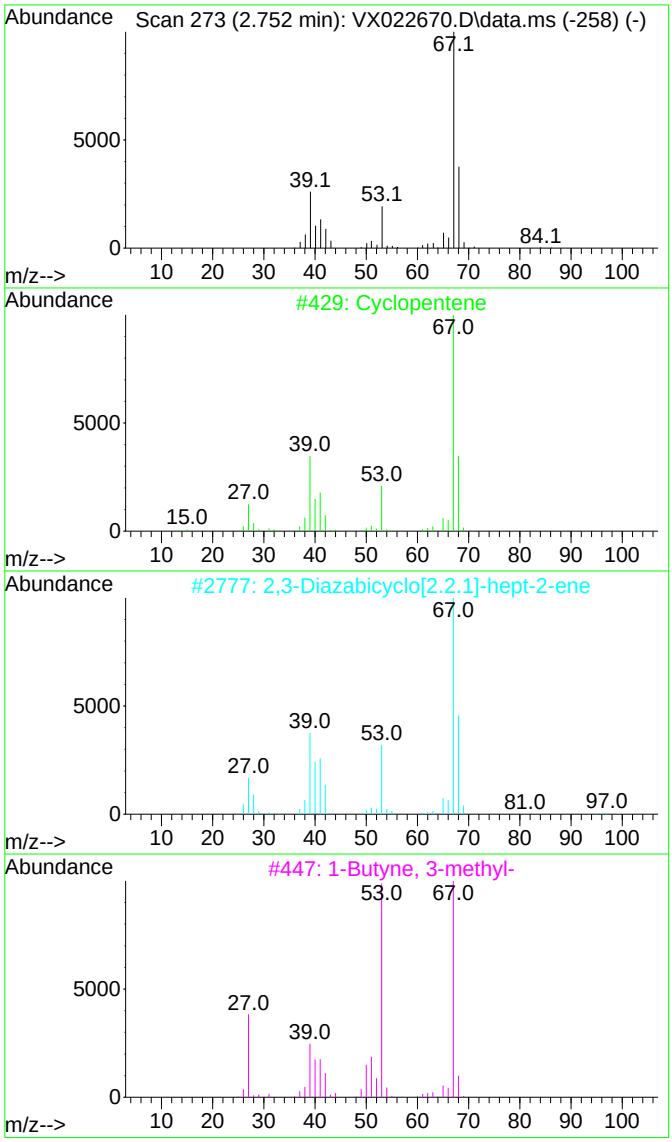
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061021W.M
Quant Title : SW846 8260

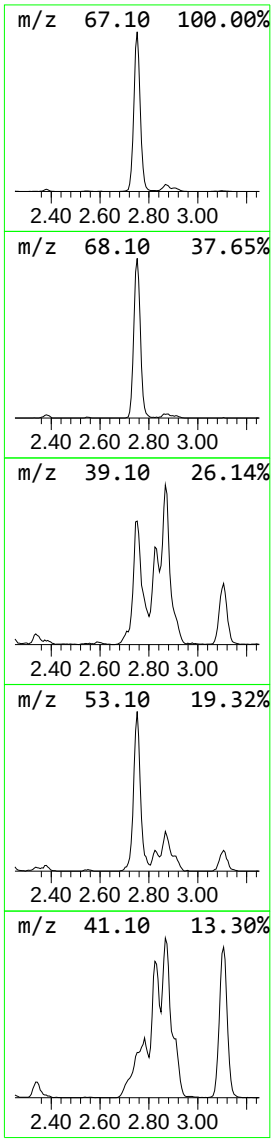
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Cyclopentene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.752	157.78 ug/l	868958	Pentafluorobenzene	5.568

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentene	68	C5H8	000142-29-0	91
2	2,3-Diazabicyclo[2.2.1]-hept-2-ene	96	C5H8N2	002721-32-6	78
3	1-Butyne, 3-methyl-	68	C5H8	000598-23-2	72
4	1,4-Pentadiene	68	C5H8	000591-93-5	58
5	1,3-Pentadiene, (Z)-	68	C5H8	001574-41-0	53





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061121\
Data File : VX022670.D
Acq On : 11 Jun 2021 16:19
Operator : JC/MD
Sample : M2688-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-2

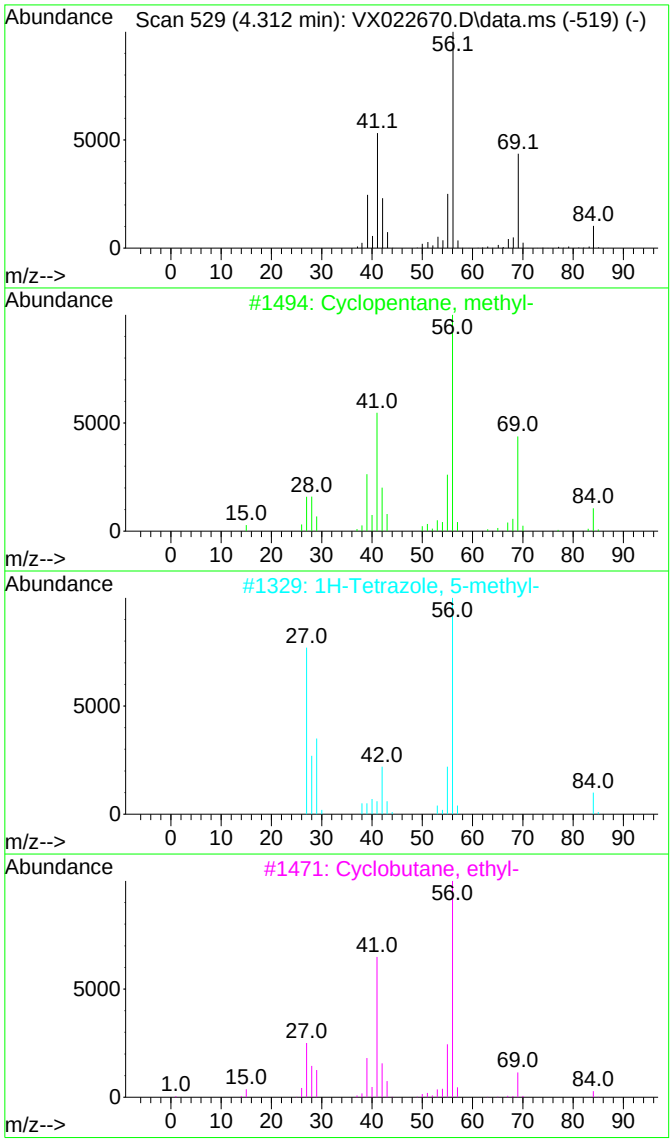
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061021W.M
Quant Title : SW846 8260

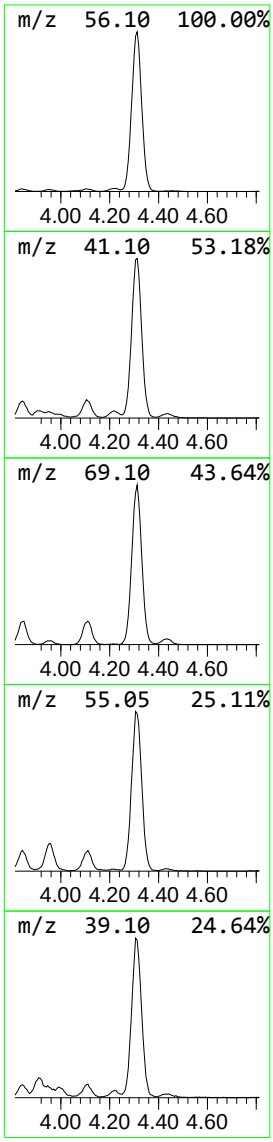
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.312	373.67 ug/l	2057990	Pentafluorobenzene	5.568

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	72
3	Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
4	Cyclohexane	84	C6H12	000110-82-7	56
5	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	47





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061121\
Data File : VX022670.D
Acq On : 11 Jun 2021 16:19
Operator : JC/MD
Sample : M2688-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-2

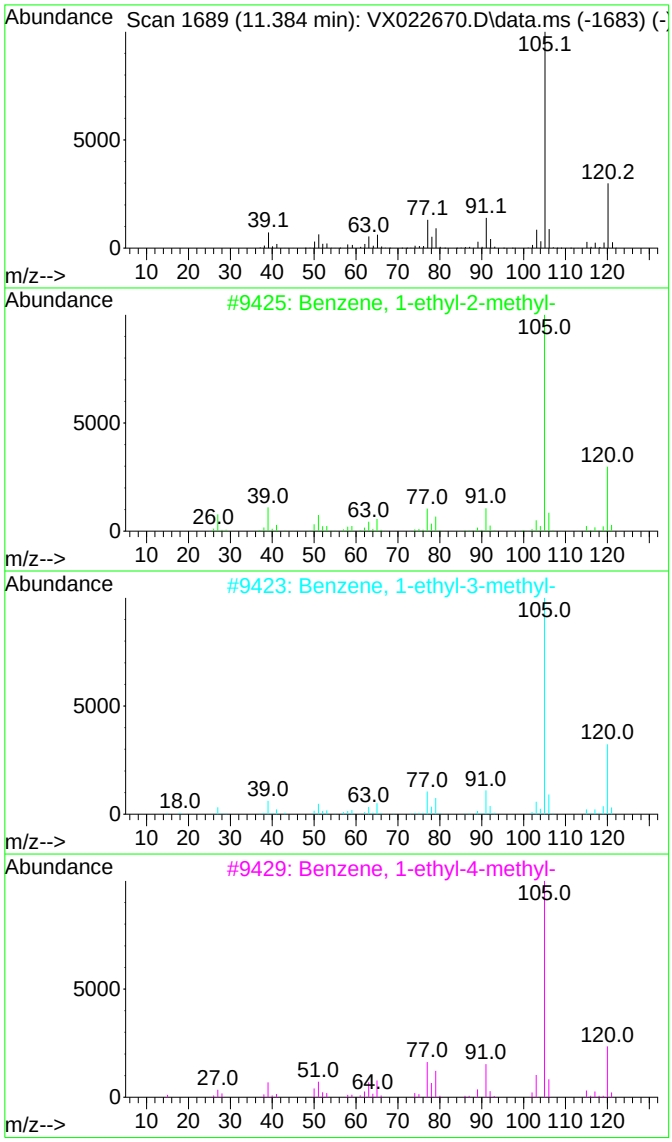
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061021W.M
Quant Title : SW846 8260

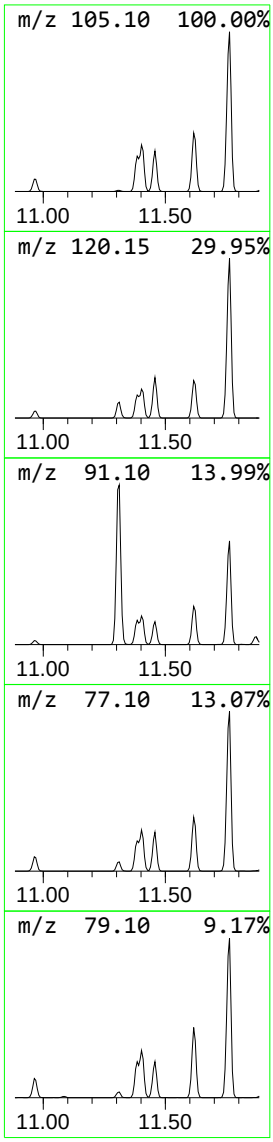
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Benzene, 1-ethyl-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.384	249.44 ug/l	2148090	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-3-methyl-	120	C9H12	000620-14-4	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	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91





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Operator : JC/MD
Sample : M2688-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-2

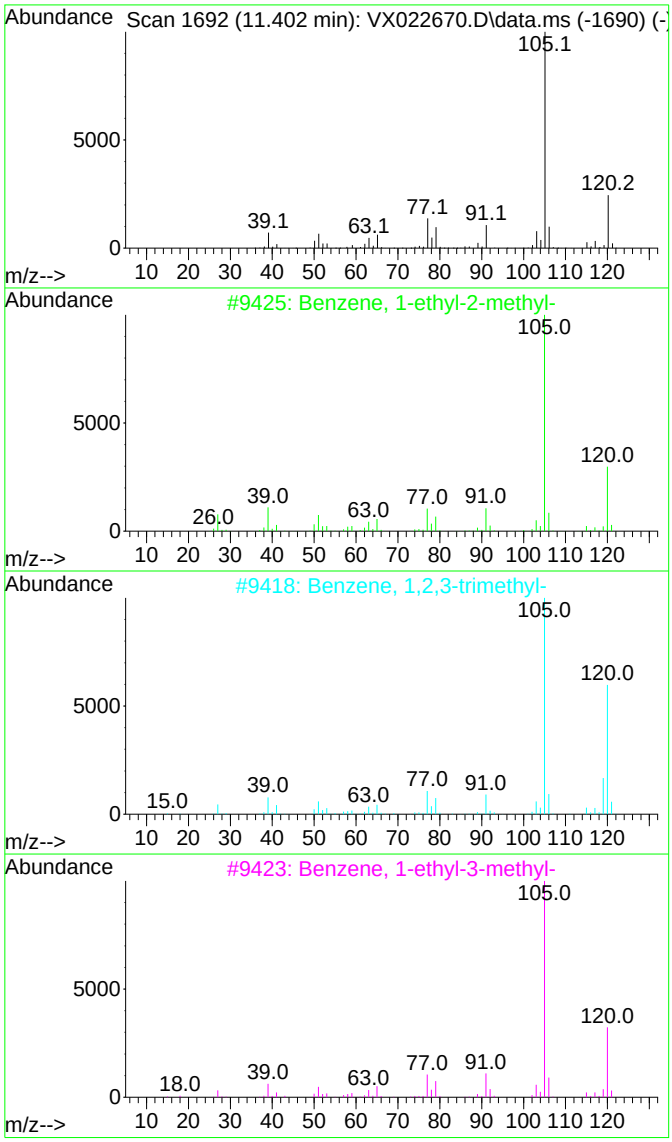
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061021W.M
Quant Title : SW846 8260

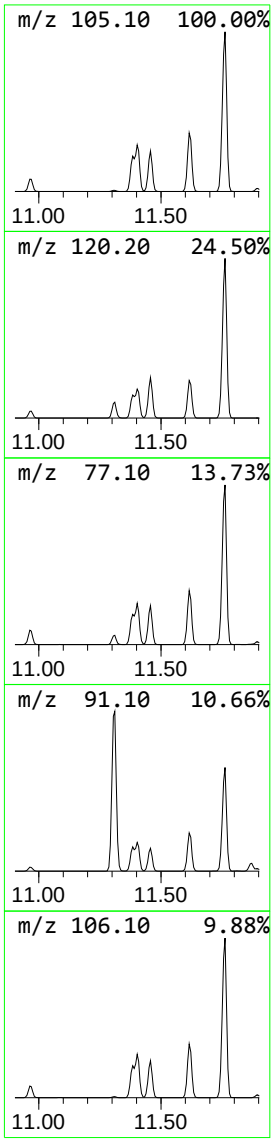
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzene, 1-ethyl-3-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.403	319.19 ug/l	2748690	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	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	Mesitylene	120	C9H12	000108-67-8	91
5	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061121\
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Sample : M2688-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-2

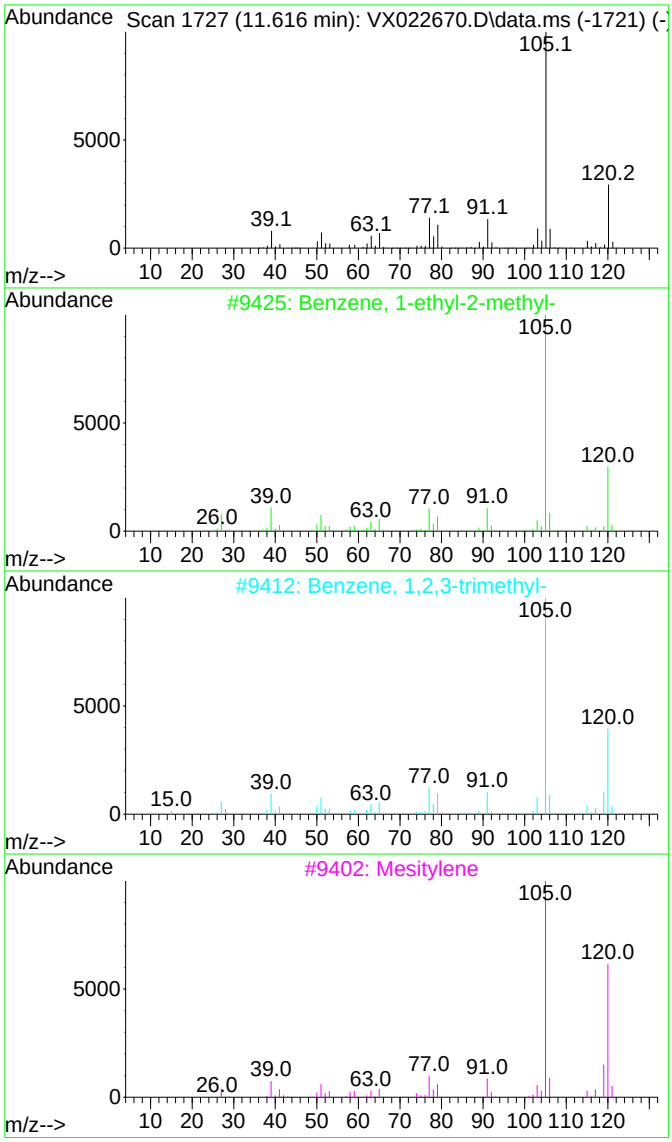
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061021W.M
Quant Title : SW846 8260

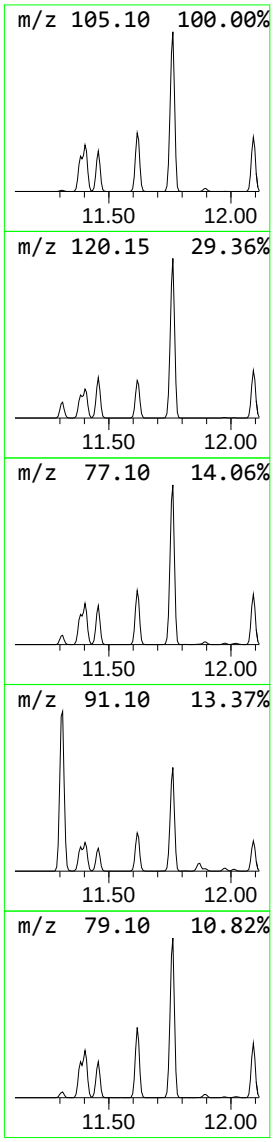
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, 1-ethyl-4-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.616	445.83 ug/l	3839270	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, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
3	Mesitylene	120	C9H12	000108-67-8	91
4	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061121\
Data File : VX022670.D
Acq On : 11 Jun 2021 16:19
Operator : JC/MD
Sample : M2688-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-2

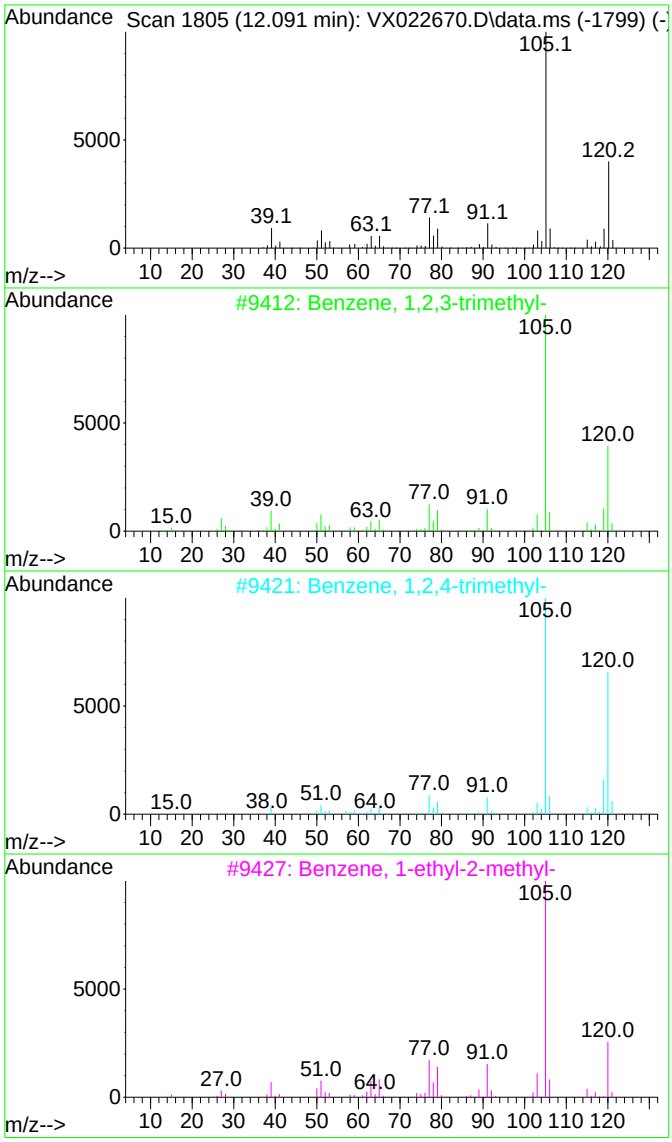
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061021W.M
Quant Title : SW846 8260

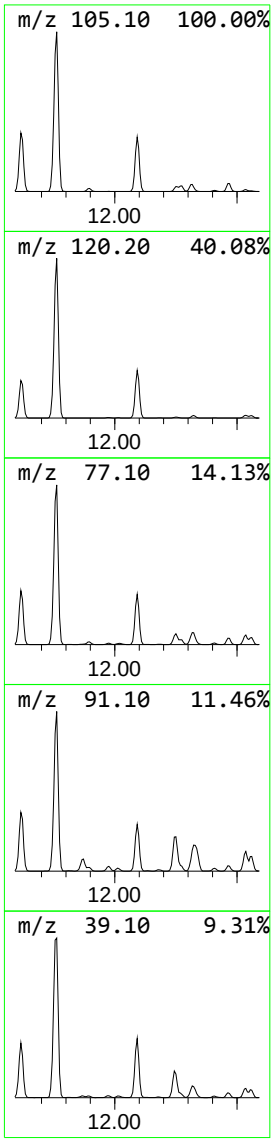
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.091	435.42 ug/l	3749600	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	97
2	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	94
3	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
4	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5	Mesitylene	120	C9H12	000108-67-8	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061121\
Data File : VX022670.D
Acq On : 11 Jun 2021 16:19
Operator : JC/MD
Sample : M2688-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-2

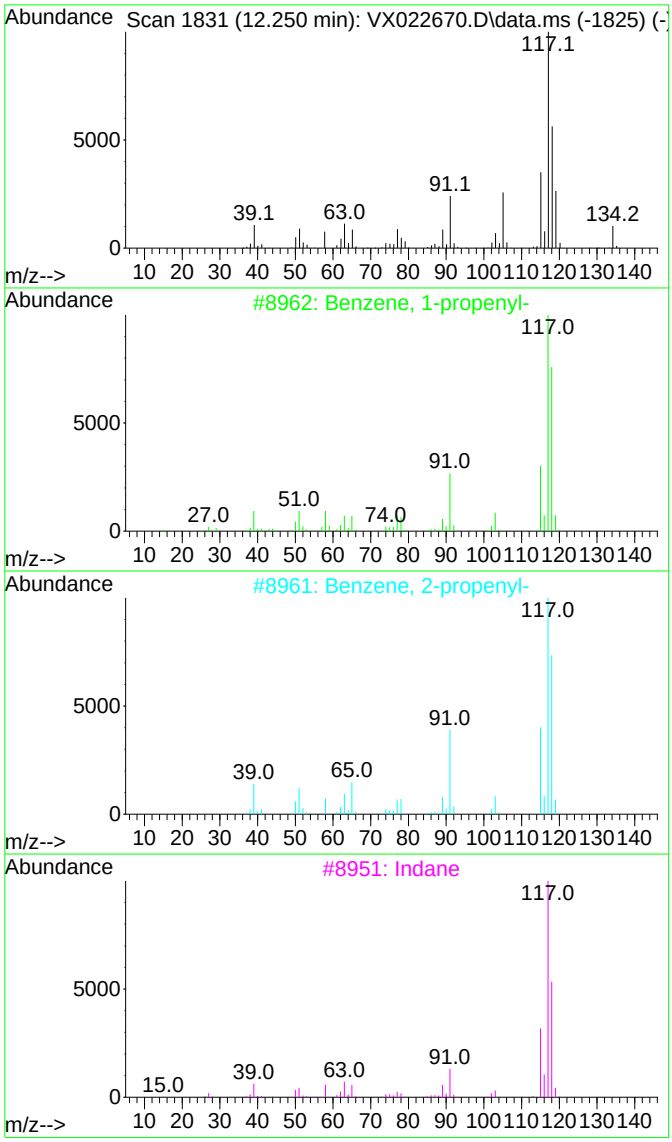
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061021W.M
Quant Title : SW846 8260

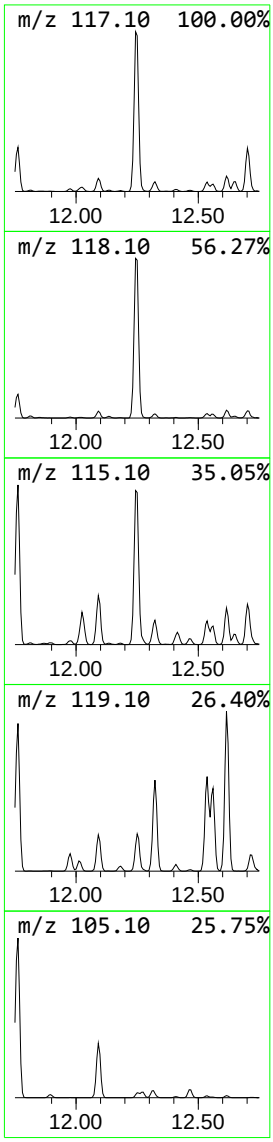
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, 1-propenyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.250	279.63 ug/l	2408080	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-propenyl-	118	C9H10	000637-50-3	91
2	Benzene, 2-propenyl-	118	C9H10	000300-57-2	70
3	Indane	118	C9H10	000496-11-7	64
4	Benzene, cyclopropyl-	118	C9H10	000873-49-4	64
5	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061121\
Data File : VX022670.D
Acq On : 11 Jun 2021 16:19
Operator : JC/MD
Sample : M2688-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-2

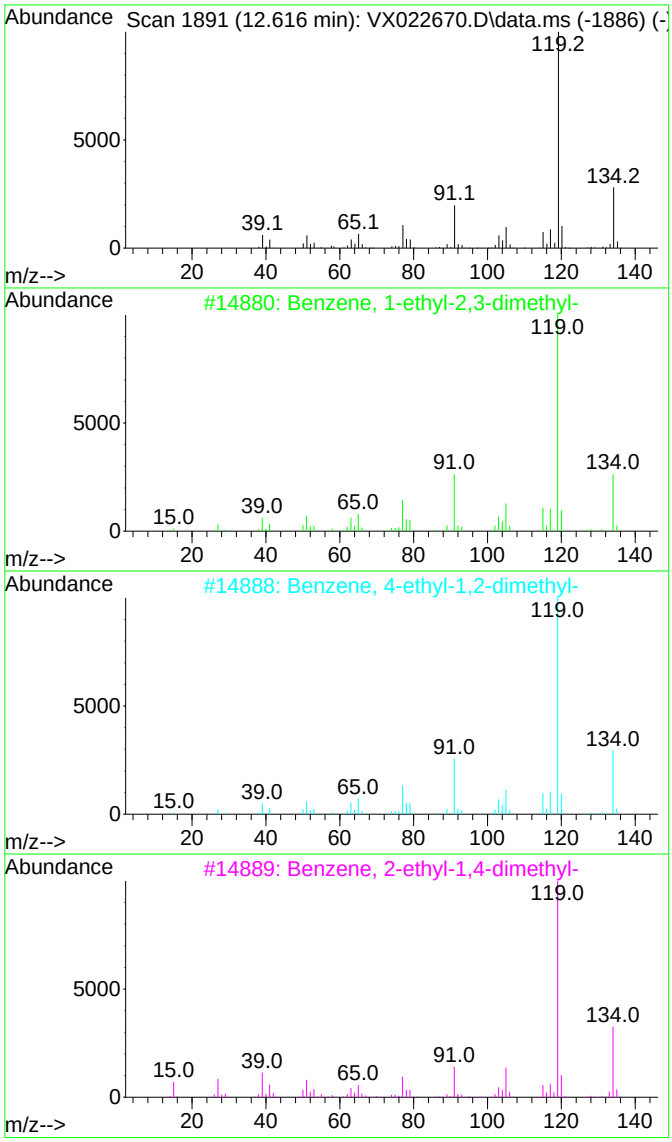
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061021W.M
Quant Title : SW846 8260

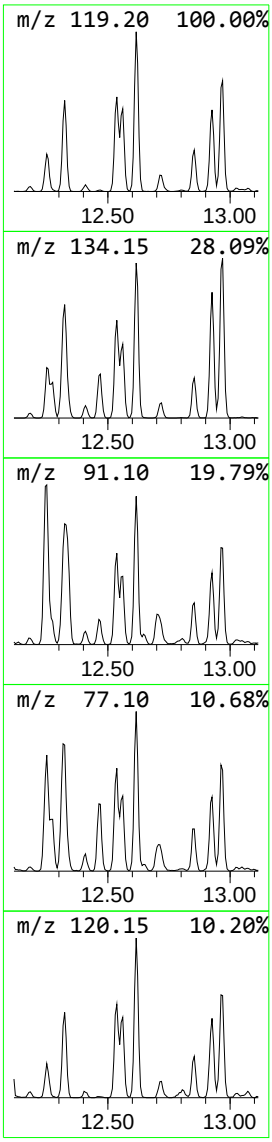
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Benzene, 1-ethyl-2,3-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.616	162.38 ug/l	1398350	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	96
2	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	96
3	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	95
4	p-Cymene	134	C10H14	000099-87-6	95
5	o-Cymene	134	C10H14	000527-84-4	95





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061121\
Data File : VX022670.D
Acq On : 11 Jun 2021 16:19
Operator : JC/MD
Sample : M2688-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061021W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methyl-	1.746	254.6	ug/l	1401960	1	5.568	275372	50.0
Pentane	1.953	168.2	ug/l	926358	1	5.568	275372	50.0
Cyclopentene	2.752	157.8	ug/l	868958	1	5.568	275372	50.0
Cyclopentane, m...	4.312	373.7	ug/l	2057990	1	5.568	275372	50.0
Benzene, 1-ethy...	11.384	249.4	ug/l	2148090	4	12.024	430578	50.0
Benzene, 1-ethy...	11.403	319.2	ug/l	2748690	4	12.024	430578	50.0
Benzene, 1-ethy...	11.616	445.8	ug/l	3839270	4	12.024	430578	50.0
Benzene, 1,2,3-...	12.091	435.4	ug/l	3749600	4	12.024	430578	50.0
Benzene, 1-prop...	12.250	279.6	ug/l	2408080	4	12.024	430578	50.0
Benzene, 1-ethy...	12.616	162.4	ug/l	1398350	4	12.024	430578	50.0