LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061121\
Data File : VX022668.D
Acq On : 11 Jun 2021 15:32
Operator : JC/MD
Sample : M2688-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-3

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: VX022668.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.751	103	109	121	rVB	432759	610678	5.38%	1.182%
2	1.953	138	142	155	rVB	360947	516551	4.55%	1.000%
3	2.068	155	161	168	rVV	117912	163972	1.44%	0.317%
4	2.215	181	185	195	rVB	76969	117173	1.03%	0.227%
5	2.782	258	278	281	rBV4	109739	354683	3.12%	0.686%
6	2.830	281	286	289	rVV	295983	611411	5.38%	1.183%
7	2.867	289	292	313	rVB2	201855	492000	4.33%	0.952%
8	3.105	319	331	348	rVB	233047	523012	4.61%	1.012%
9	3.446	378	387	401	rBV	197423	440655	3.88%	0.853%
10	4.312	518	529	543	rVB	697463	2007626	17.68%	3.885%
11	5.397	696	707	711	rBV2	42870	124209	1.09%	0.240%
12	5.482	711	721	730	rVV	669660	2131048	18.77%	4.123%
13	5.556	731	733	741	rVV2	76226	199428	1.76%	0.386%
14	5.836	767	779	792	rBV4	51697	172396	1.52%	0.334%
15	5.964	792	800	806	rVV	55141	142391	1.25%	0.276%
16	6.049	806	814	824	rVV	246854	655243	5.77%	1.268%
17	6.165	824	833	842	rVV4	66875	280188	2.47%	0.542%
18	6.257	843	848	857	rVV4	97502	289819	2.55%	0.561%
19	6.360	857	865	878	rVB	72010	201910	1.78%	0.391%
20	6.769	923	932	941	rBV	127031	313829	2.76%	0.607%
21	7.384	1021	1033	1043	rBV2	304747	756421	6.66%	1.464%
22	8.110	1144	1152	1156	rBV	57943	129067	1.14%	0.250%
23	8.506	1211	1217	1225	rVB2	74111	129474	1.14%	0.251%
24	8.653	1236	1241	1246	rVB	260150	398097	3.51%	0.770%
25	8.726	1246	1253	1260	rBV	2625612	4070964	35.85%	7.877%
26	10.055	1460	1471	1477	rBV	256269	365308	3.22%	0.707%
27	10.201	1489	1495	1506	rBV	2900438	3891147	34.27%	7.529%
28	10.311	1506	1513	1527	rVB	7816793	11355372	100.00%	21.972%
29	10.646	1562	1568	1579	rVB	4557588	5998354	52.82%	11.607%
30	10.963	1614	1620	1626	rVB	176369	226272	1.99%	0.438%
31	11.085	1635	1640	1645	rBV	208361	259476	2.29%	0.502%
32	11.305	1668	1676	1683	rBV	343691	446643	3.93%	0.864%
33	11.384	1683	1689	1696	rVV	1587263	2705431	23.83%	5.235%
34	11.457	1696	1701	1712	rVB	731815	923280	8.13%	1.787%
35	11.615	1722	1727	1735	rVB	911161	1101168	9.70%	2.131%
36	11.756	1745	1750	1755	rBV	2897764	3461884	30.49%	6.699%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061121\
Data File : VX022668.D
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Operator : JC/MD
Sample : M2688-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-3

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	12.024	1789	1794	1799	rVB	284166	351674	3.10%	0.680%
38	12.091	1799	1805	1810	rBV	990098	1163477	10.25%	2.251%
39	12.243	1825	1830	1838	rBV2	730507	1091286	9.61%	2.112%
40	12.323	1838	1843	1850	rVB2	215574	306384	2.70%	0.593%
41	12.536	1872	1878	1880	rBV	122308	171240	1.51%	0.331%
42	12.615	1886	1891	1894	rBV	210447	245701	2.16%	0.475%
43	12.701	1900	1905	1913	rVB2	132570	200910	1.77%	0.389%
44	12.926	1935	1942	1945	rBV	119643	152412	1.34%	0.295%
45	12.963	1945	1948	1954	rVB	191795	236284	2.08%	0.457%
46	13.170	1978	1982	1987	rVB	114939	137634	1.21%	0.266%
47	13.292	1998	2002	2008	rVB2	252242	349074	3.07%	0.675%
48	13.780	2076	2082	2087	rBV	573013	707959	6.23%	1.370%

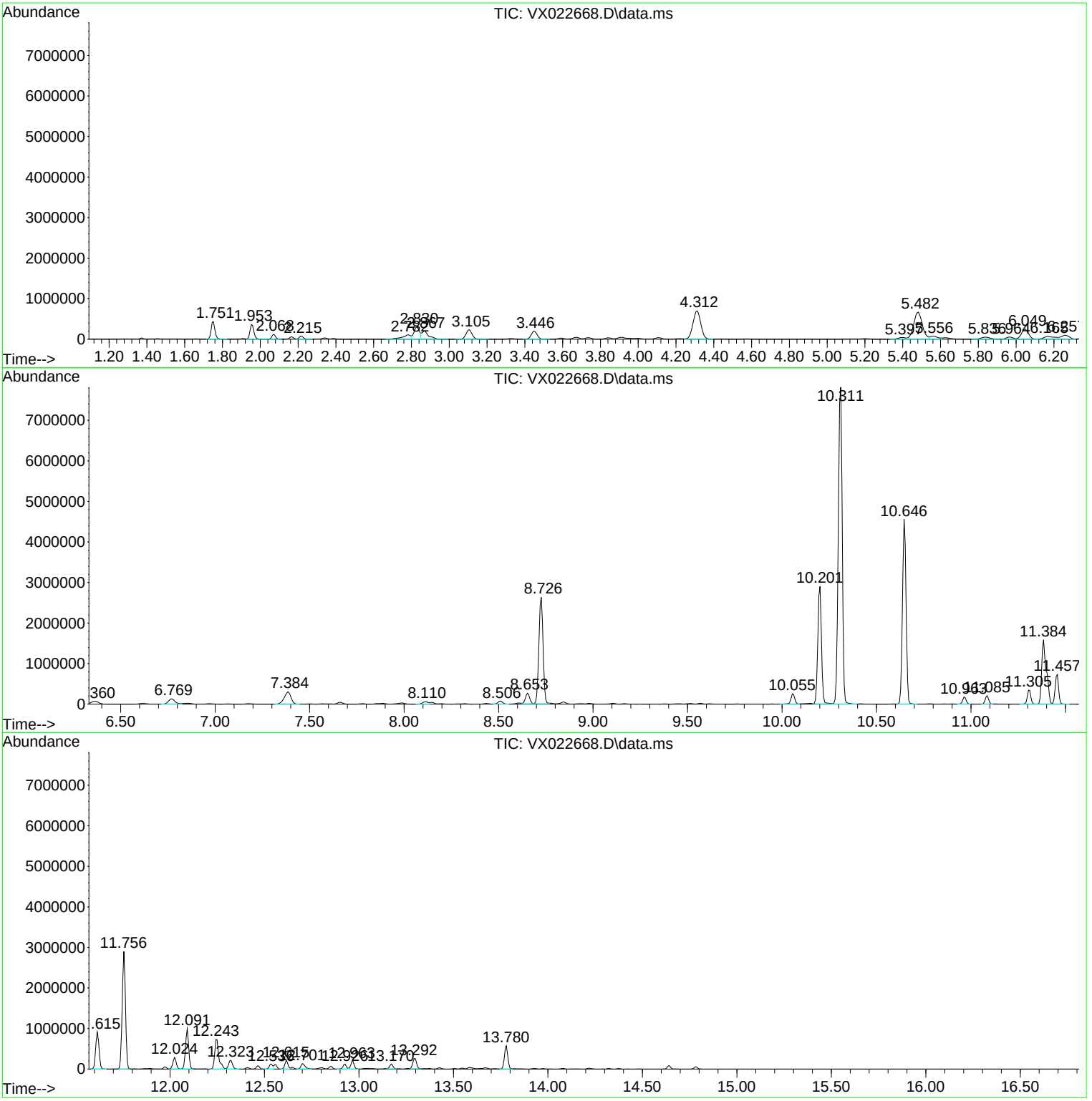
Sum of corrected areas: 51680615

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061121\
Data File : VX022668.D
Acq On : 11 Jun 2021 15:32
Operator : JC/MD
Sample : M2688-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3

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 : VX022668.D
Acq On : 11 Jun 2021 15:32
Operator : JC/MD
Sample : M2688-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3

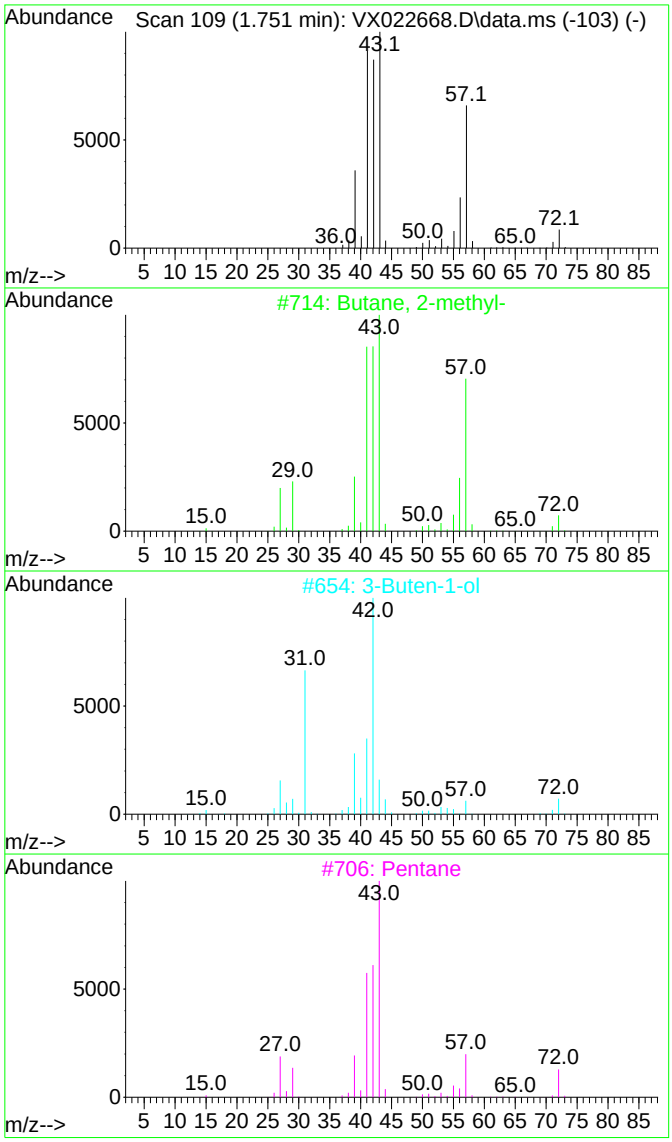
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061021W.M
Quant Title : SW846 8260

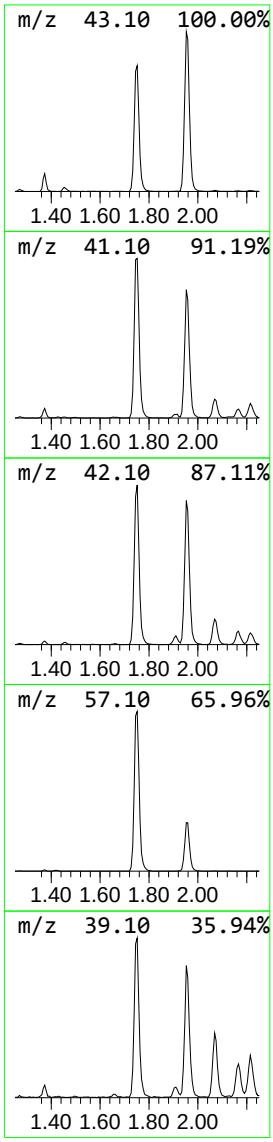
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Butane, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.751	153.11 ug/l	610678	Pentafluorobenzene	5.562

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	Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	16
5	1-Propene, 2-methyl-	56	C4H8	000115-11-7	10





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061121\
Data File : VX022668.D
Acq On : 11 Jun 2021 15:32
Operator : JC/MD
Sample : M2688-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3

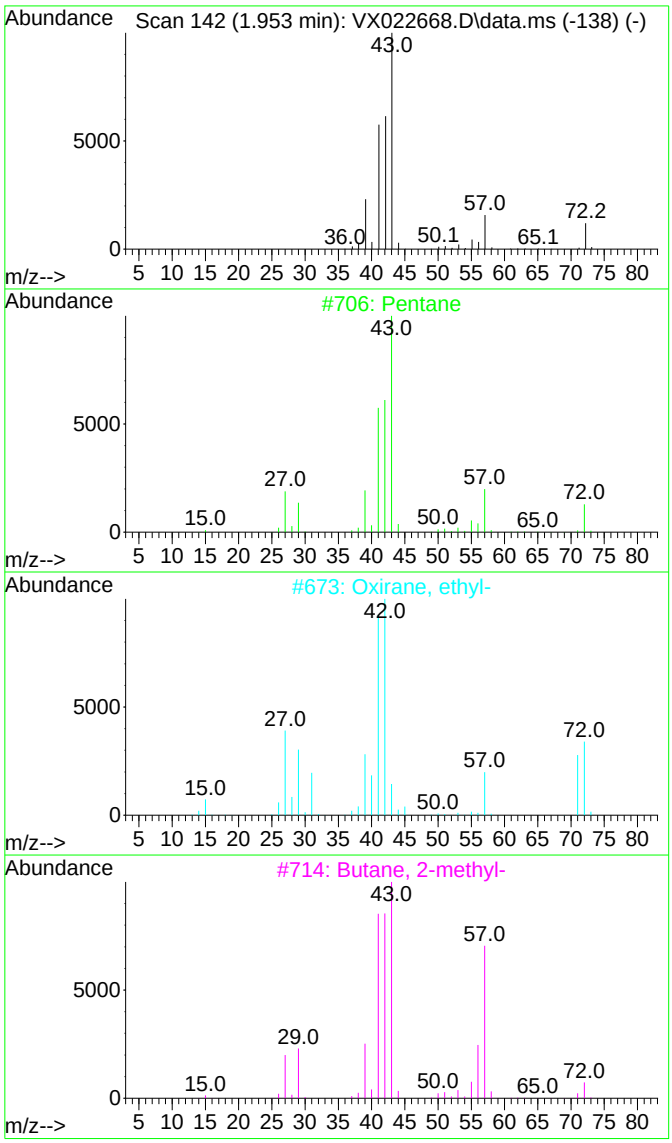
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061021W.M
Quant Title : SW846 8260

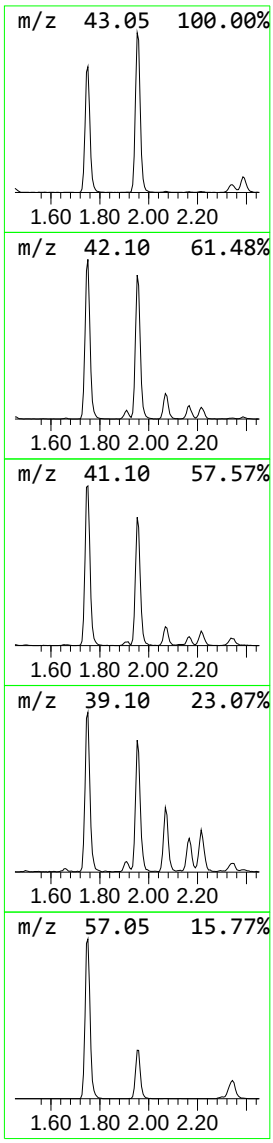
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Pentane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.953	129.51 ug/l	516551	Pentafluorobenzene	5.562

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	53
3	Butane, 2-methyl-	72	C5H12	000078-78-4	36
4	Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	35
5	Isobutylene epoxide	72	C4H8O	000558-30-5	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061121\
Data File : VX022668.D
Acq On : 11 Jun 2021 15:32
Operator : JC/MD
Sample : M2688-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3

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

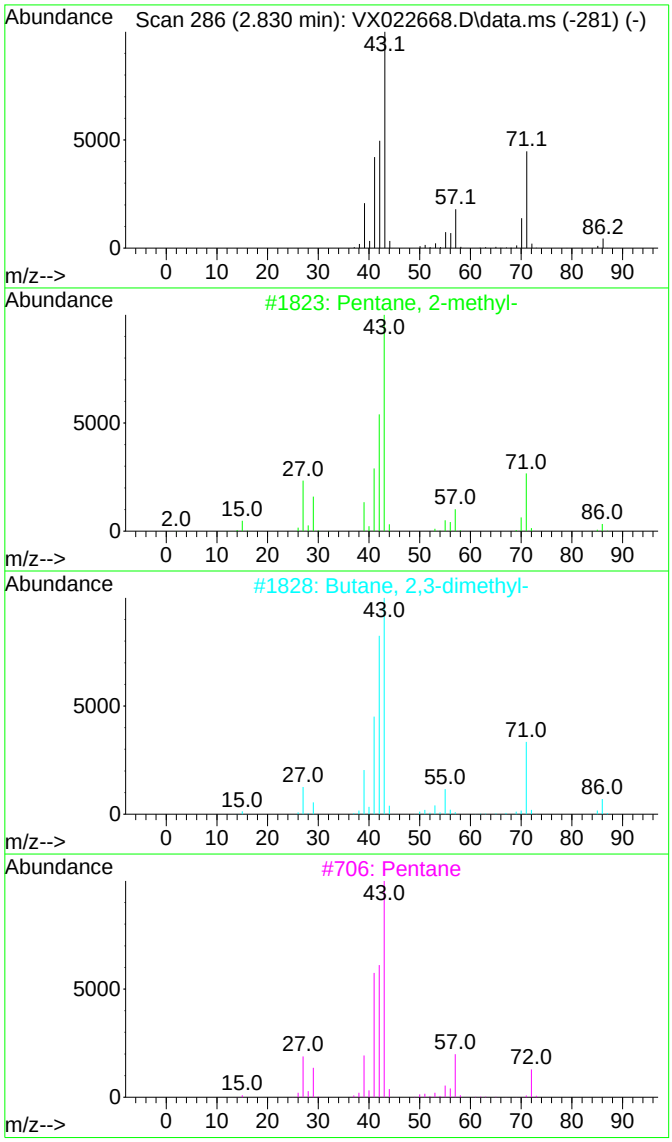
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

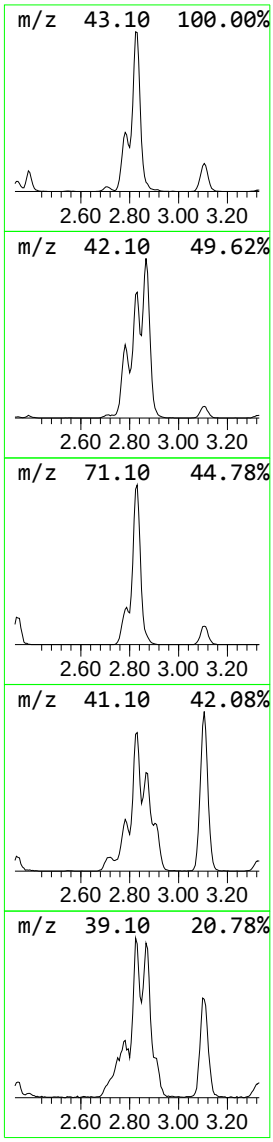
****

Peak Number 3 Pentane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.830	153.29 ug/l	611411	Pentafluorobenzene	5.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2-methyl-	86	C6H14	000107-83-5	91
2	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	46
3	Pentane	72	C5H12	000109-66-0	43
4	Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	28
5	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	23





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061121\
Data File : VX022668.D
Acq On : 11 Jun 2021 15:32
Operator : JC/MD
Sample : M2688-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3

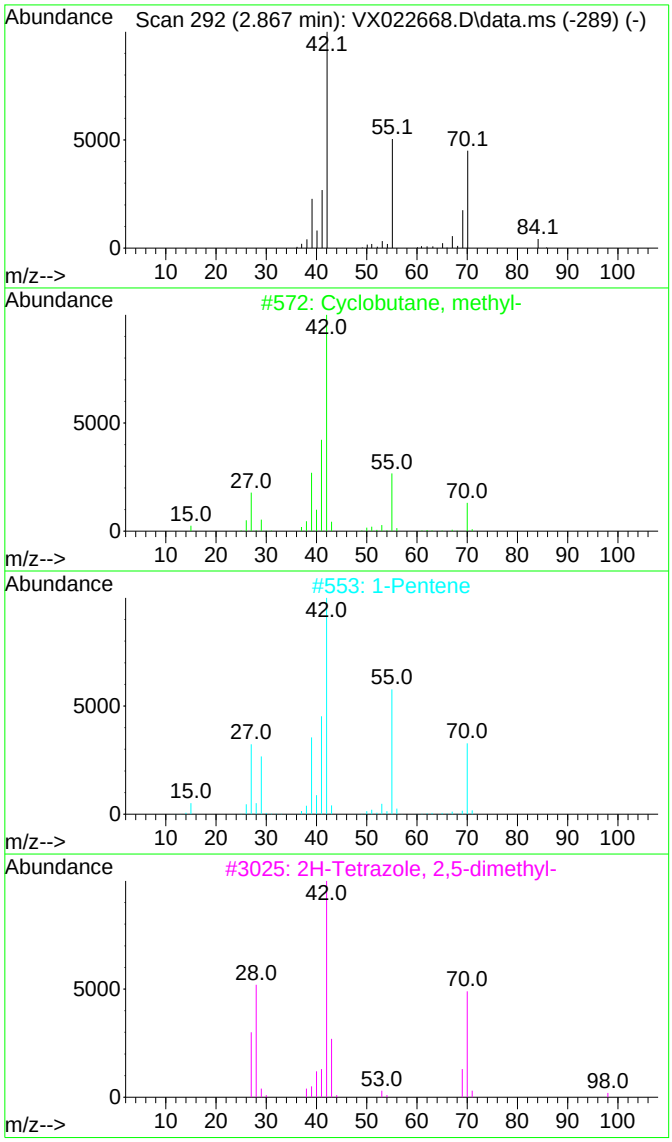
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061021W.M
Quant Title : SW846 8260

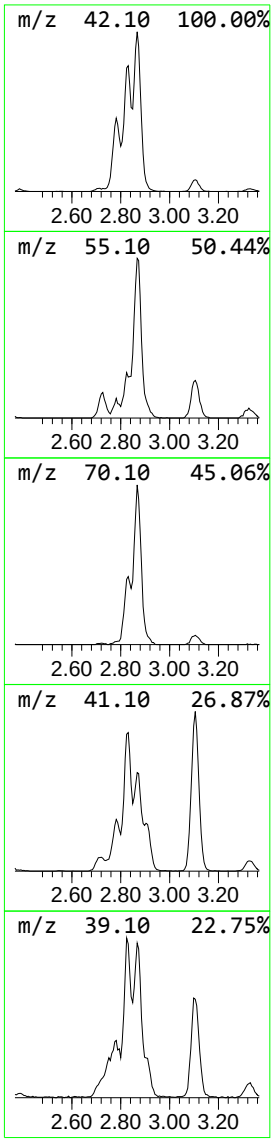
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Cyclobutane, methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.867	123.35 ug/l	492000	Pentafluorobenzene	5.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclobutane, methyl-	70	C5H10	000598-61-8	72
2	1-Pentene	70	C5H10	000109-67-1	50
3	2H-Tetrazole, 2,5-dimethyl-	98	C3H6N4	004135-93-7	39
4	2-Pentene	70	C5H10	000109-68-2	37
5	2-Pentene, (Z)-	70	C5H10	000627-20-3	37





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061121\
Data File : VX022668.D
Acq On : 11 Jun 2021 15:32
Operator : JC/MD
Sample : M2688-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3

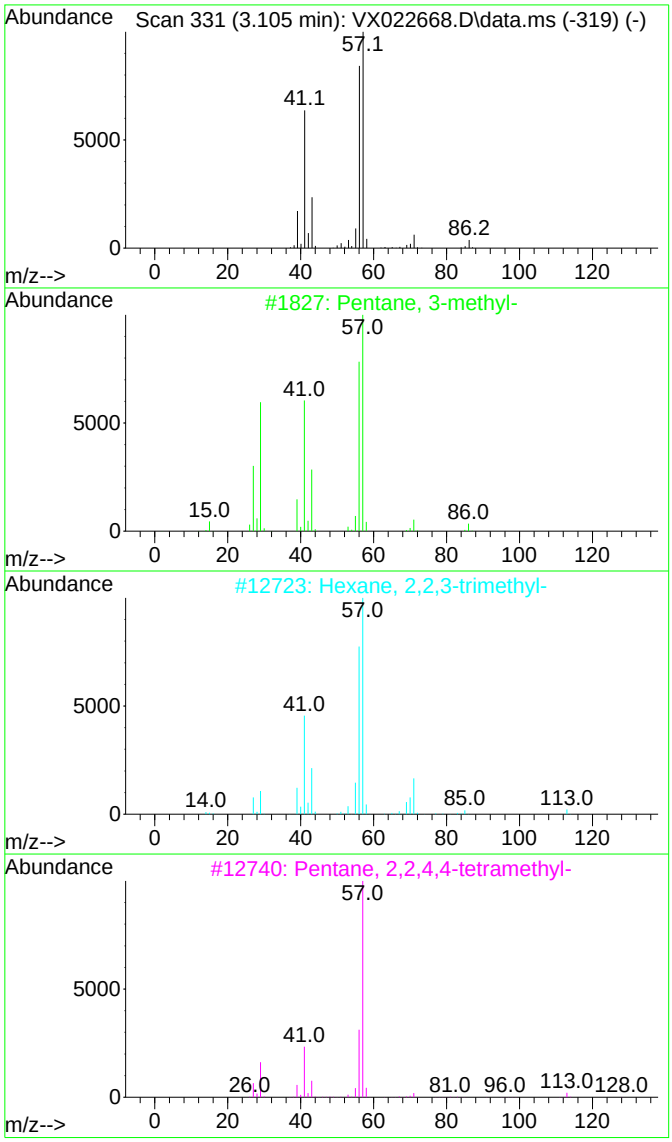
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061021W.M
Quant Title : SW846 8260

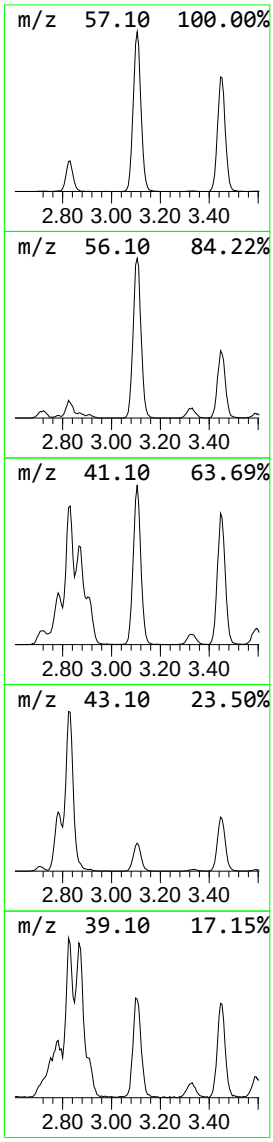
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Pentane, 3-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.105	131.13 ug/l	523012	Pentafluorobenzene	5.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 3-methyl-	86	C6H14	000096-14-0	91
2	Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	78
3	Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	45
4	Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	43
5	Butyl isocyanatoacetate	157	C7H11NO3	017046-22-9	40





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061121\
Data File : VX022668.D
Acq On : 11 Jun 2021 15:32
Operator : JC/MD
Sample : M2688-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3

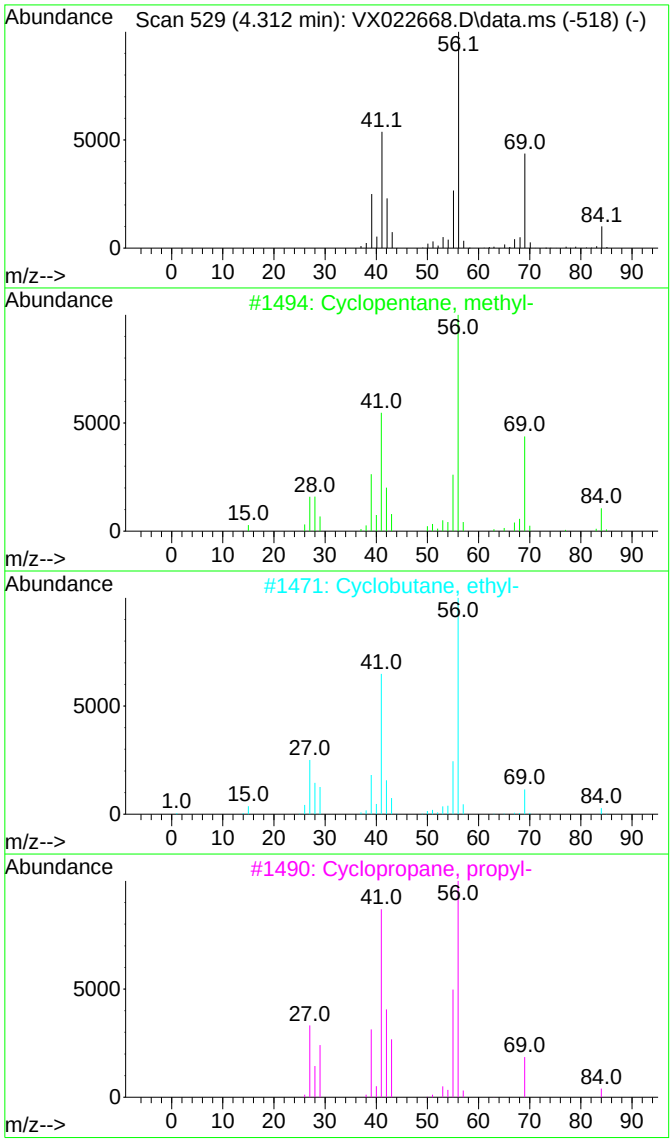
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061021W.M
Quant Title : SW846 8260

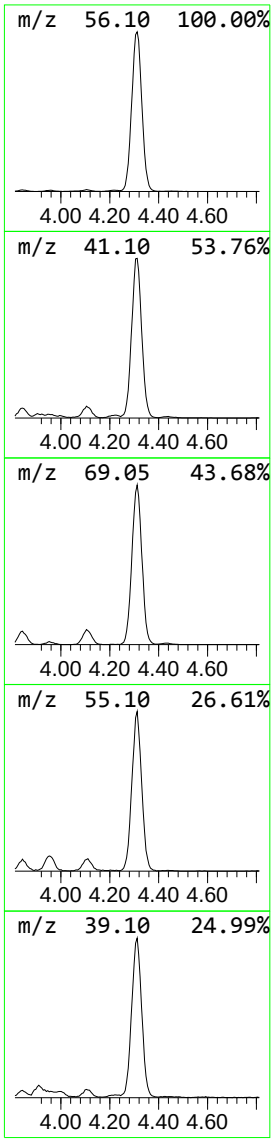
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Cyclopentane, methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.312	503.35 ug/l	2007630	Pentafluorobenzene	5.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2	Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
3	Cyclopropane, propyl-	84	C6H12	002415-72-7	56
4	Cyclohexane	84	C6H12	000110-82-7	56
5	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	56





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Data File : VX022668.D
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Operator : JC/MD
Sample : M2688-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3

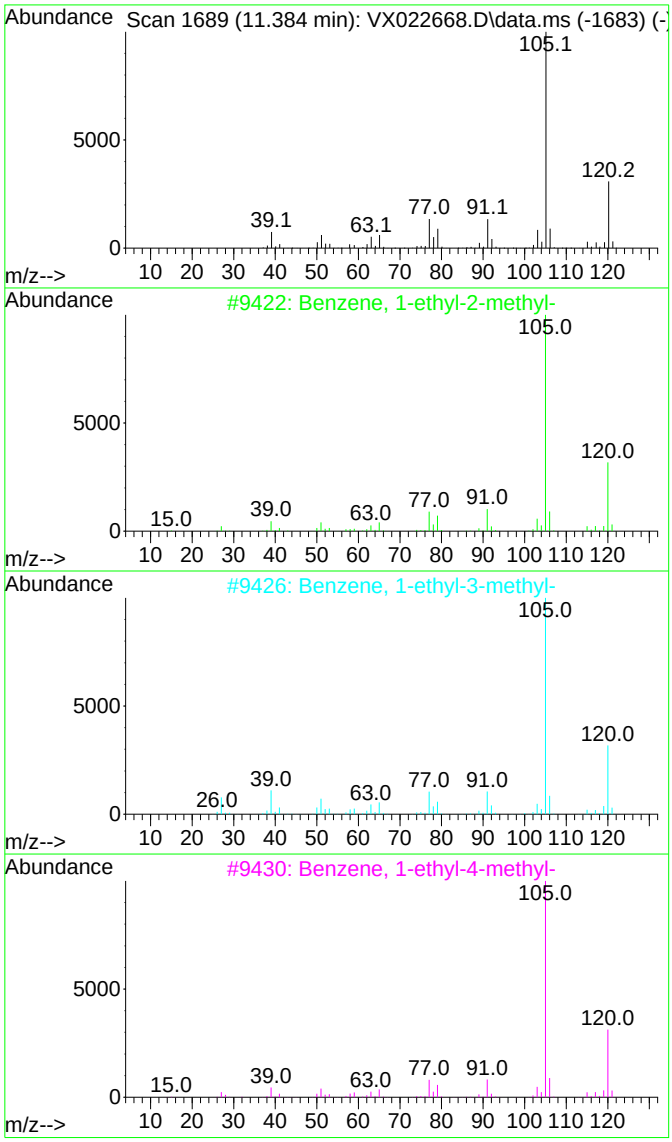
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061021W.M
Quant Title : SW846 8260

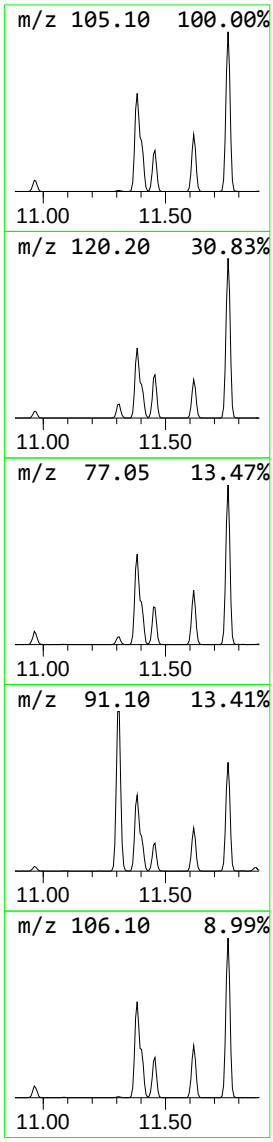
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.384	384.65 ug/l	2705430	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	Mesitylene	120	C9H12	000108-67-8	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061121\
Data File : VX022668.D
Acq On : 11 Jun 2021 15:32
Operator : JC/MD
Sample : M2688-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3

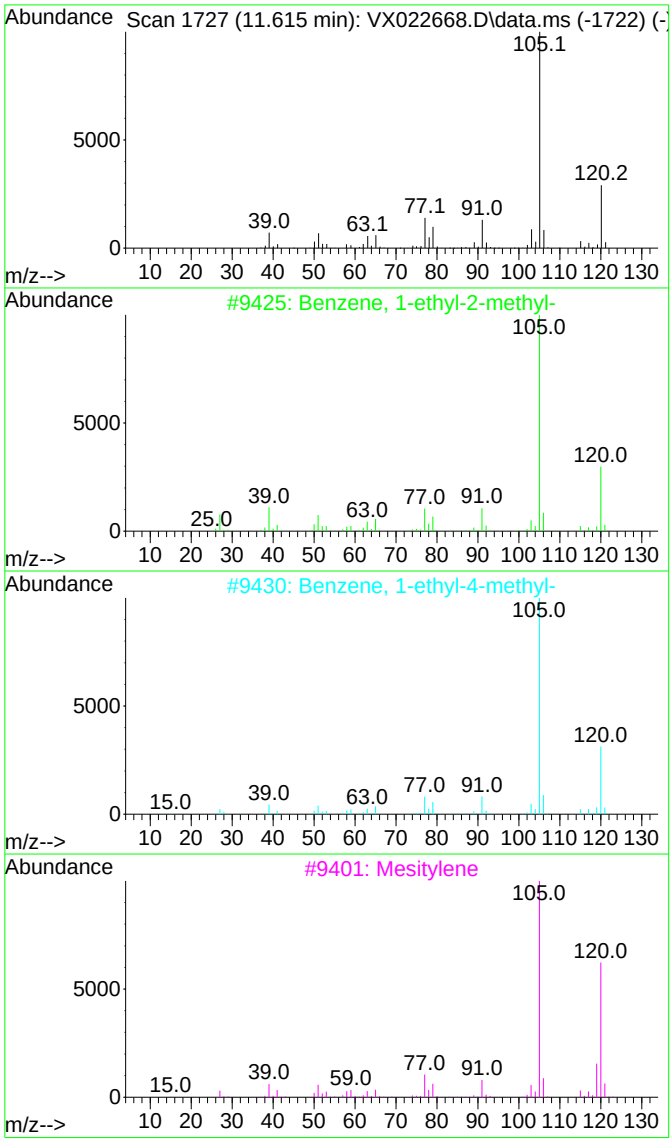
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061021W.M
Quant Title : SW846 8260

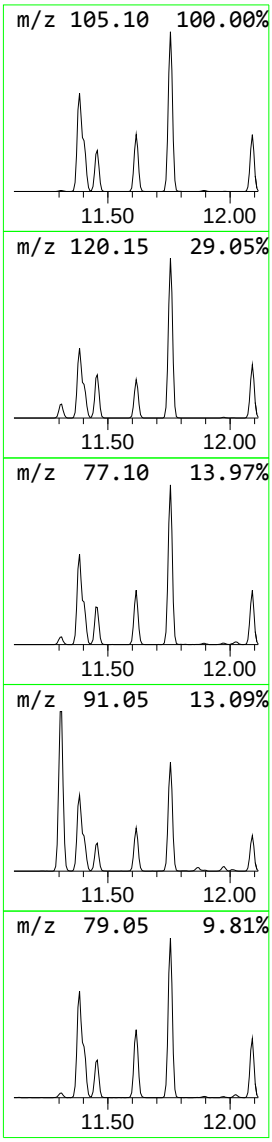
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, 1-ethyl-4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.615	156.56 ug/l	1101170	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	91
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





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061121\
Data File : VX022668.D
Acq On : 11 Jun 2021 15:32
Operator : JC/MD
Sample : M2688-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3

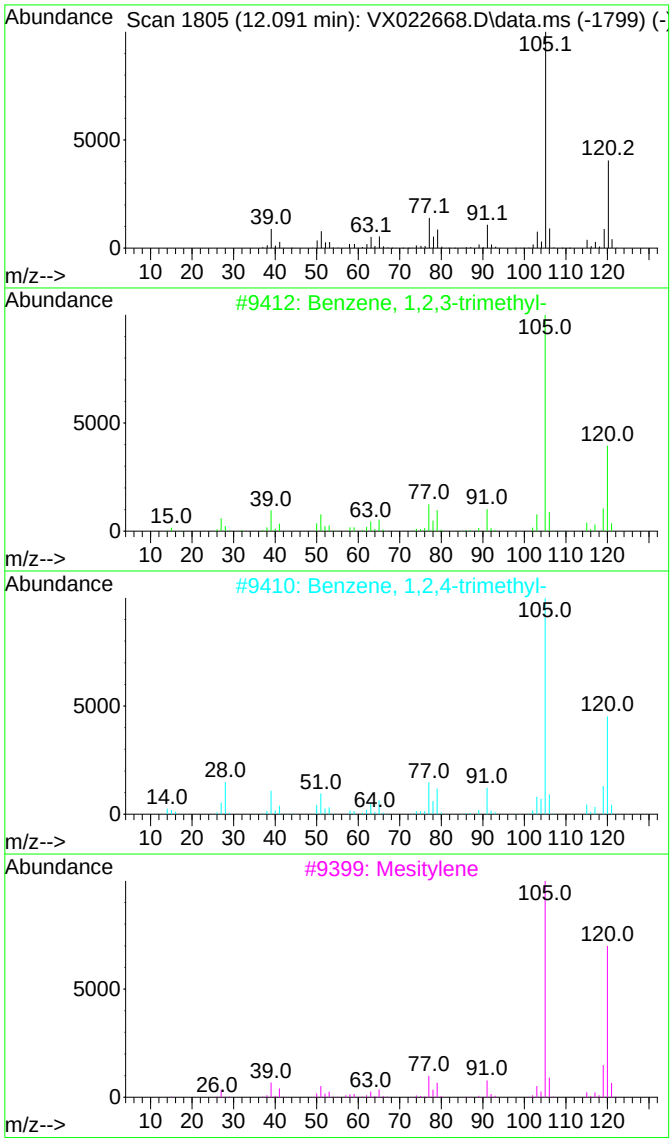
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061021W.M
Quant Title : SW846 8260

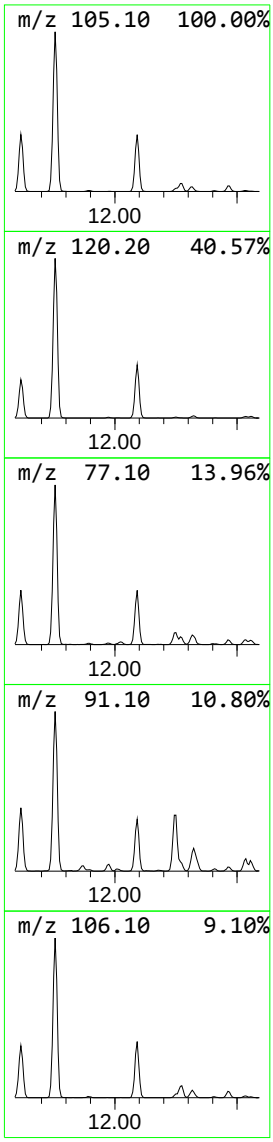
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.091	165.42 ug/l	1163480	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	Mesitylene	120	C9H12	000108-67-8	94
4	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	93
5	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061121\
Data File : VX022668.D
Acq On : 11 Jun 2021 15:32
Operator : JC/MD
Sample : M2688-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-3

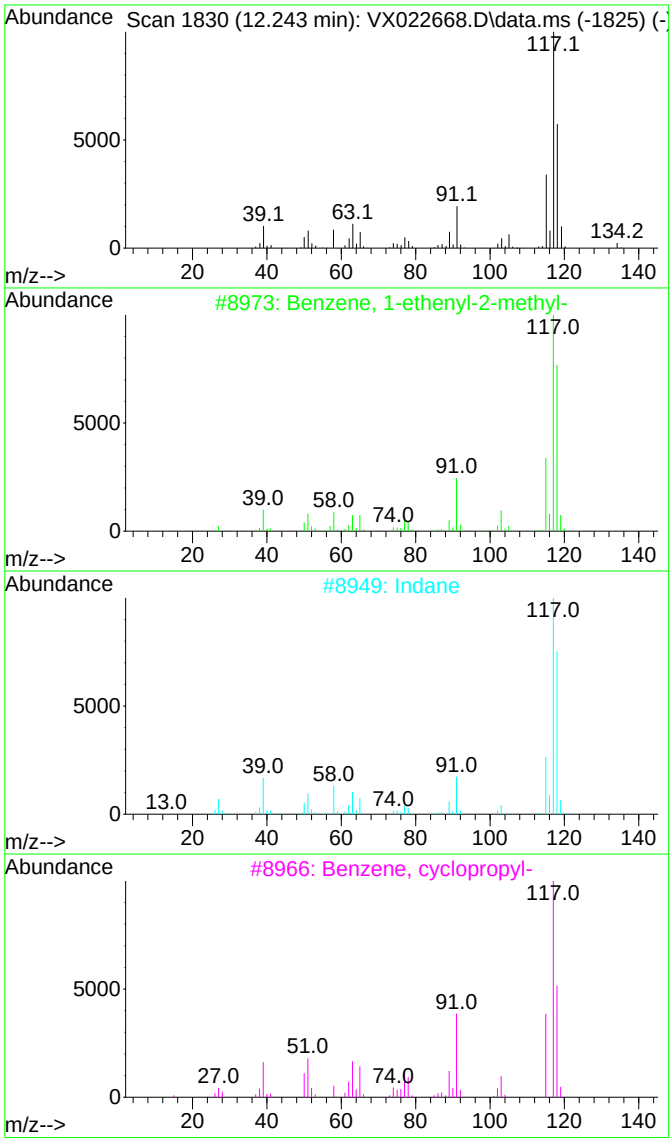
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061021W.M
Quant Title : SW846 8260

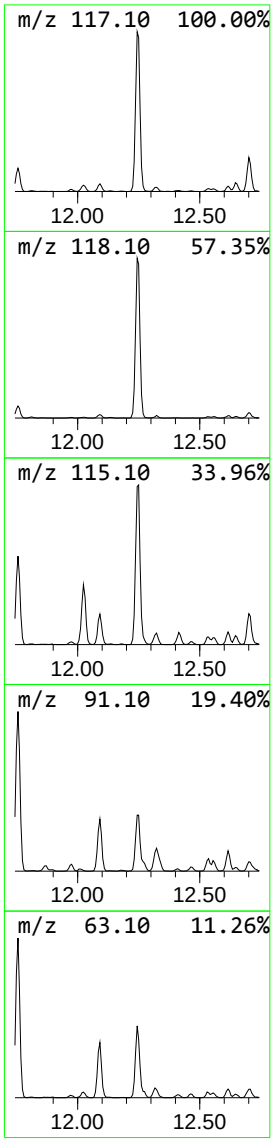
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Benzene, 1-ethenyl-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.243	155.16 ug/l	1091290	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	89
2	Indane	118	C9H10	000496-11-7	87
3	Benzene, cyclopropyl-	118	C9H10	000873-49-4	81
4	Benzene, 2-propenyl-	118	C9H10	000300-57-2	81
5	Benzene, 1-propenyl-	118	C9H10	000637-50-3	68





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061121\
Data File : VX022668.D
Acq On : 11 Jun 2021 15:32
Operator : JC/MD
Sample : M2688-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-3

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-	1.751	153.1	ug/l	610678	1	5.562	199428	50.0
Pentane	1.953	129.5	ug/l	516551	1	5.562	199428	50.0
Pentane, 2-methyl-	2.830	153.3	ug/l	611411	1	5.562	199428	50.0
Cyclobutane, me...	2.867	123.3	ug/l	492000	1	5.562	199428	50.0
Pentane, 3-methyl-	3.105	131.1	ug/l	523012	1	5.562	199428	50.0
Cyclopentane, m...	4.312	503.4	ug/l	2007630	1	5.562	199428	50.0
Benzene, 1-ethy...	11.384	384.6	ug/l	2705430	4	12.024	351674	50.0
Benzene, 1-ethy...	11.615	156.6	ug/l	1101170	4	12.024	351674	50.0
Benzene, 1,2,3-...	12.091	165.4	ug/l	1163480	4	12.024	351674	50.0
Benzene, 1-ethe...	12.243	155.2	ug/l	1091290	4	12.024	351674	50.0