LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090222\
Data File : VN074311.D
Acq On : 03 Sep 2022 01:51
Operator : JC\MD
Sample : N4355-07
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 34 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP082322

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_N\methods\82N090222W.M
Title : SW846 8260

Signal : TIC: VN074311.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.405	79	88	97	rBV	2973725	4531560	1.71%	0.421%
2	3.087	193	204	229	rVB	18246290	38746778	14.63%	3.601%
3	3.457	258	267	289	rVV	3694587	9028745	3.41%	0.839%
4	3.934	339	348	362	rVB	1134730	2997961	1.13%	0.279%
5	5.081	533	543	576	rVB5	2364144	13981756	5.28%	1.299%
6	5.534	604	620	639	rBV	1788332	6169878	2.33%	0.573%
7	6.040	692	706	722	rBV2	1141296	3416190	1.29%	0.317%
8	7.069	869	881	905	rVB	8885021	26062586	9.84%	2.422%
9	8.022	1034	1043	1052	rBV2	6983002	17565607	6.63%	1.632%
10	8.392	1096	1106	1114	rBV3	1427663	3796540	1.43%	0.353%
11	8.510	1114	1126	1132	rVV5	1252008	4164087	1.57%	0.387%
12	8.904	1183	1193	1200	rBV2	1519640	3856126	1.46%	0.358%
13	9.392	1261	1276	1294	rBV	3905414	10167286	3.84%	0.945%
14	10.380	1436	1444	1449	rBV	1609669	3020802	1.14%	0.281%
15	10.445	1449	1455	1460	rVV	4512408	7808707	2.95%	0.726%
16	11.686	1658	1666	1672	rBV	1649652	2949613	1.11%	0.274%
17	11.786	1675	1683	1693	rVV2	62076747	97194531	36.69%	9.033%
18	11.898	1693	1702	1713	rVV4	136516408	264927008	100.00%	24.621%
19	12.222	1745	1757	1773	rVB	30308659	48475396	18.30%	4.505%
20	12.516	1796	1807	1816	rBV	3592843	5767234	2.18%	0.536%
21	12.857	1858	1865	1870	rBV	9810440	15391593	5.81%	1.430%
22	12.922	1870	1876	1879	rVV2	32759611	50383077	19.02%	4.682%
23	12.957	1879	1882	1886	rVV	19277905	28611038	10.80%	2.659%
24	12.998	1886	1889	1896	rVB	14093174	20365457	7.69%	1.893%
25	13.157	1909	1916	1928	rVB	20584377	32947752	12.44%	3.062%
26	13.310	1929	1942	1949	rBV2	107232871	158797477	59.94%	14.758%
27	13.645	1988	1999	2009	rBV	24071770	40782303	15.39%	3.790%
28	13.816	2022	2028	2033	rVV	19142868	31154876	11.76%	2.895%
29	14.004	2053	2060	2065	rBV2	1901066	3468609	1.31%	0.322%
30	14.068	2065	2071	2074	rVV	3427773	5832930	2.20%	0.542%
31	14.098	2074	2076	2081	rVV	2998431	3746305	1.41%	0.348%
32	14.157	2081	2086	2091	rVV	5377606	8217165	3.10%	0.764%
33	14.263	2100	2104	2114	rVB2	5262596	8504204	3.21%	0.790%
34	14.474	2132	2140	2144	rBV	3269963	5599065	2.11%	0.520%
35	14.516	2144	2147	2152	rVB	4791011	6661358	2.51%	0.619%
36	14.745	2181	2186	2192	rBV	4635007	6988231	2.64%	0.649%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090222\
Data File : VN074311.D
Acq On : 03 Sep 2022 01:51
Operator : JC\MD
Sample : N4355-07
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 34 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP082322

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_N\methods\82N090222W.M
Title : SW846 8260

37	14.863	2198	2206	2213	rBV2	8721008	17188809	6.49%	1.597%
38	15.015	2225	2232	2240	rBV	2285869	3967237	1.50%	0.369%
39	15.127	2240	2251	2255	rBV3	1053618	2766932	1.04%	0.257%
40	15.433	2289	2303	2310	rBV	17965965	31805638	12.01%	2.956%
41	16.527	2481	2489	2504	rVB	4925367	10998004	4.15%	1.022%
42	16.733	2515	2524	2533	rBV	3167886	7200564	2.72%	0.669%

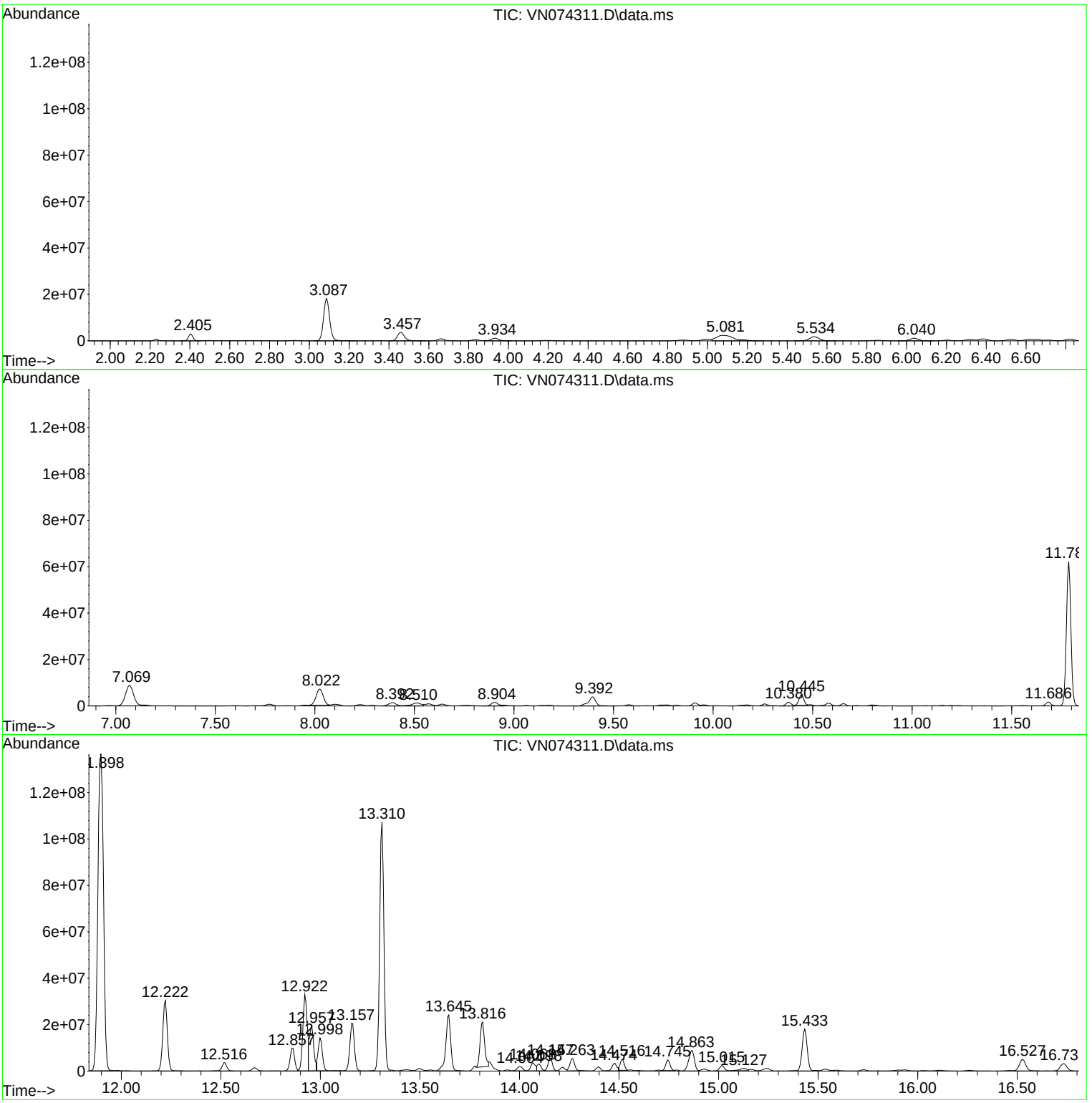
Sum of corrected areas: 1076007015

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090222\
Data File : VN074311.D
Acq On : 03 Sep 2022 01:51
Operator : JC\MD
Sample : N4355-07
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 34 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP082322

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090222W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090222\
Data File : VN074311.D
Acq On : 03 Sep 2022 01:51
Operator : JC\MD
Sample : N4355-07
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 34 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP082322

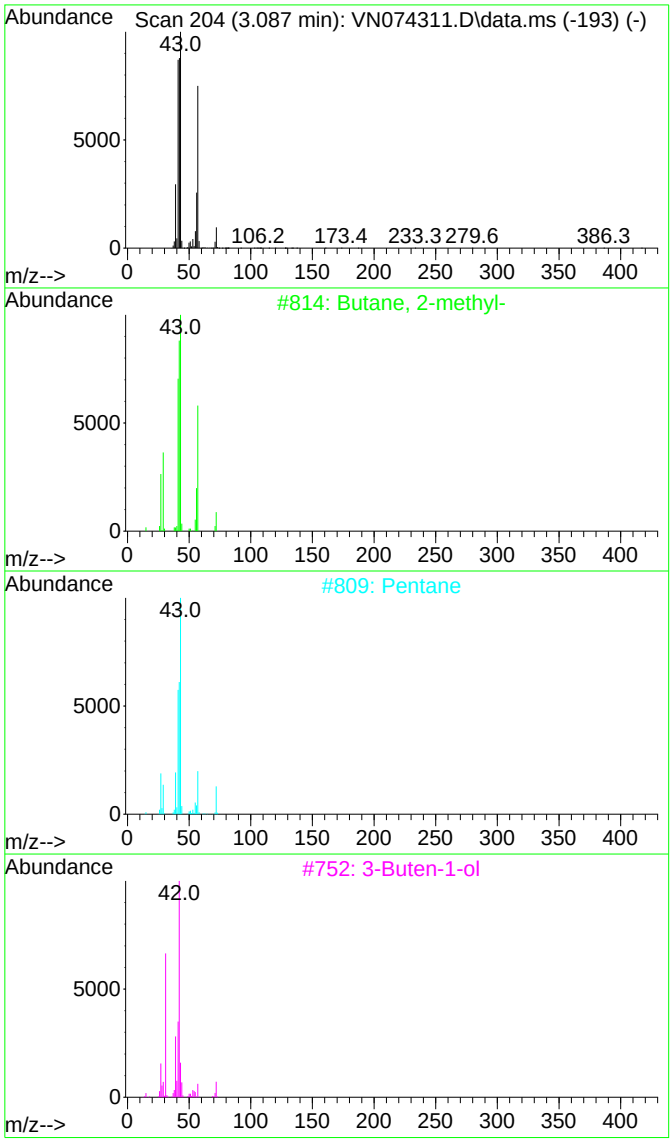
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090222W.M
Quant Title : SW846 8260

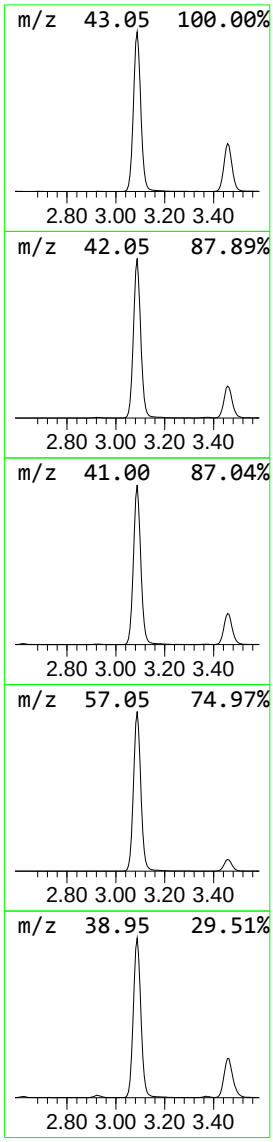
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.087	110.29 ug/l	38746800	Pentafluorobenzene	8.022

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	91
2	Pentane	72	C5H12	000109-66-0	43
3	3-Buten-1-ol	72	C4H8O	000627-27-0	25
4	Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	10
5	1-Propene, 2-methyl-	56	C4H8	000115-11-7	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090222\
Data File : VN074311.D
Acq On : 03 Sep 2022 01:51
Operator : JC\MD
Sample : N4355-07
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 34 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP082322

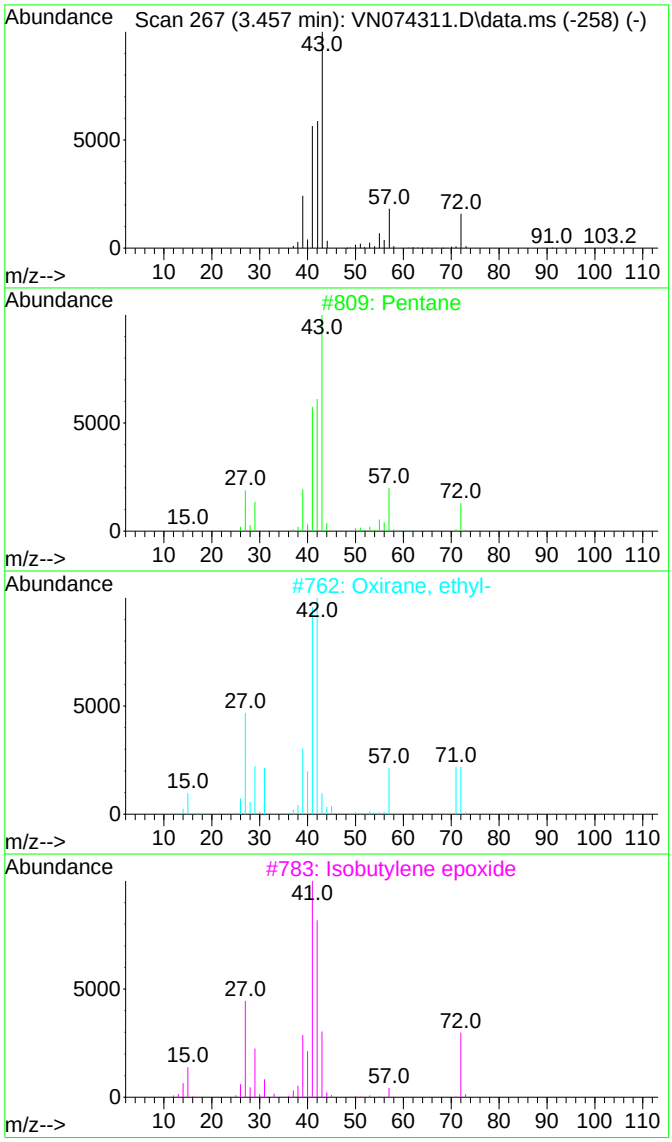
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090222W.M
Quant Title : SW846 8260

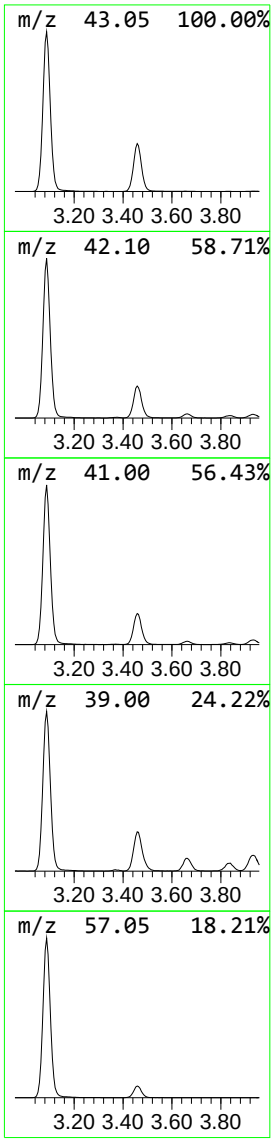
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Pentane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.457	25.70 ug/l	9028750	Pentafluorobenzene	8.022

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	50
3	Isobutylene epoxide	72	C4H8O	000558-30-5	47
4	Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	40
5	Tetrahydrofuran	72	C4H8O	000109-99-9	37





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090222\
Data File : VN074311.D
Acq On : 03 Sep 2022 01:51
Operator : JC\MD
Sample : N4355-07
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 34 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP082322

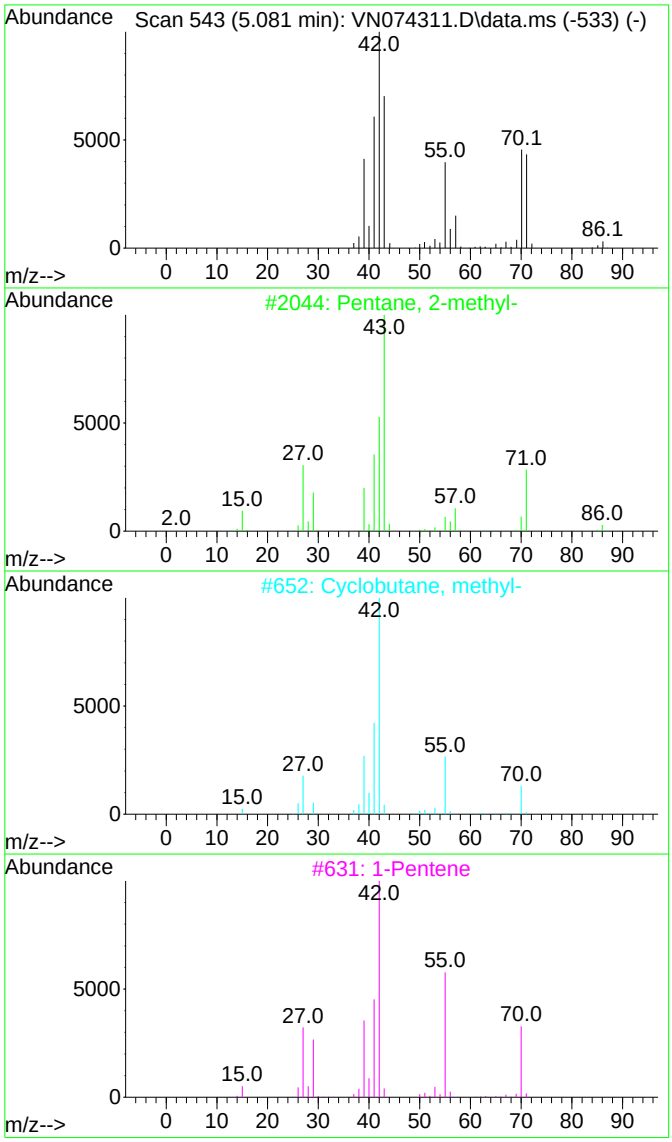
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090222W.M
Quant Title : SW846 8260

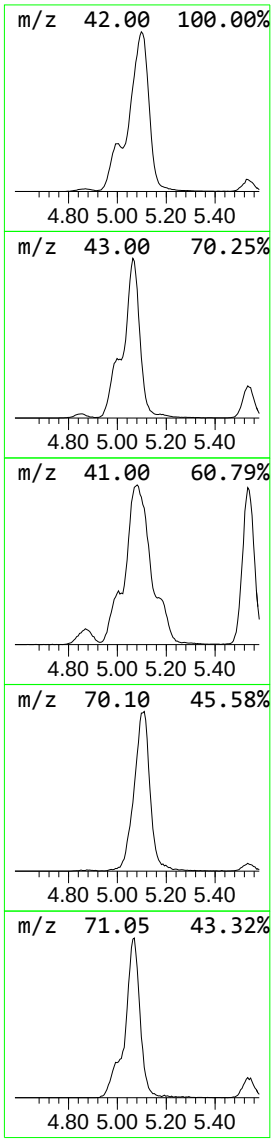
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 unknown5.081 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.081	39.80 ug/l	13981800	Pentafluorobenzene	8.022

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2-methyl-	86	C6H14	000107-83-5	45
2	Cyclobutane, methyl-	70	C5H10	000598-61-8	43
3	1-Pentene	70	C5H10	000109-67-1	43
4	Cyclopentane	70	C5H10	000287-92-3	38
5	Pentane, 1-chloro-	106	C5H11Cl	000543-59-9	37





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090222\
Data File : VN074311.D
Acq On : 03 Sep 2022 01:51
Operator : JC\MD
Sample : N4355-07
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 34 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP082322

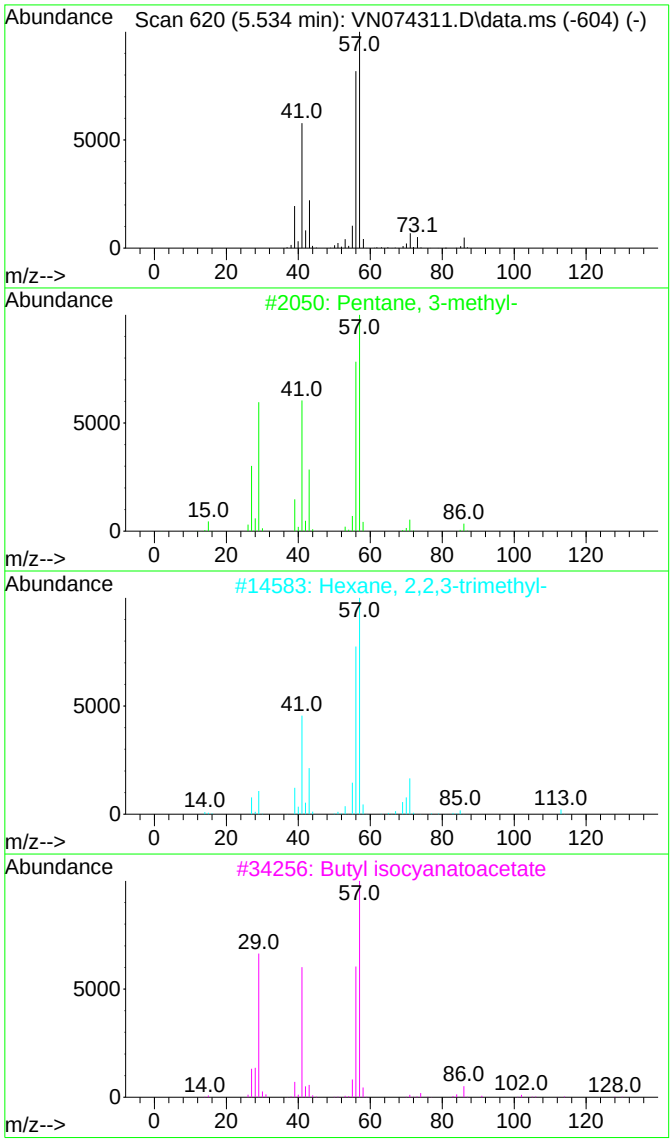
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090222W.M
Quant Title : SW846 8260

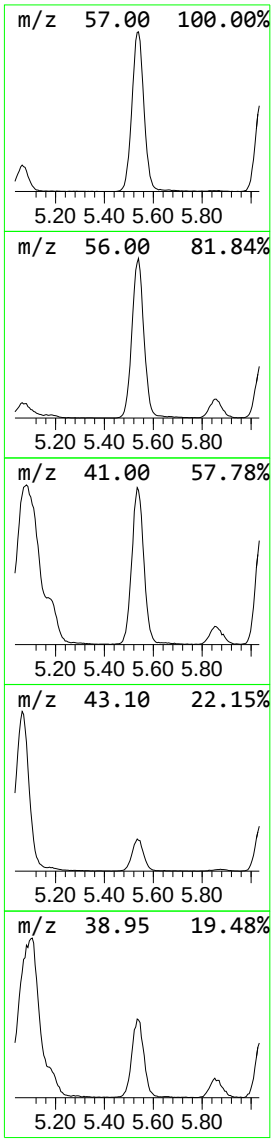
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Pentane, 3-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.534	17.56 ug/l	6169880	Pentafluorobenzene	8.022

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 3-methyl-	86	C6H14	000096-14-0	90
2	Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	78
3	Butyl isocyanatoacetate	157	C7H11NO3	017046-22-9	56
4	3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	40
5	1-Butanol, 2-methyl-	88	C5H12O	000137-32-6	40





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090222\
Data File : VN074311.D
Acq On : 03 Sep 2022 01:51
Operator : JC\MD
Sample : N4355-07
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 34 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP082322

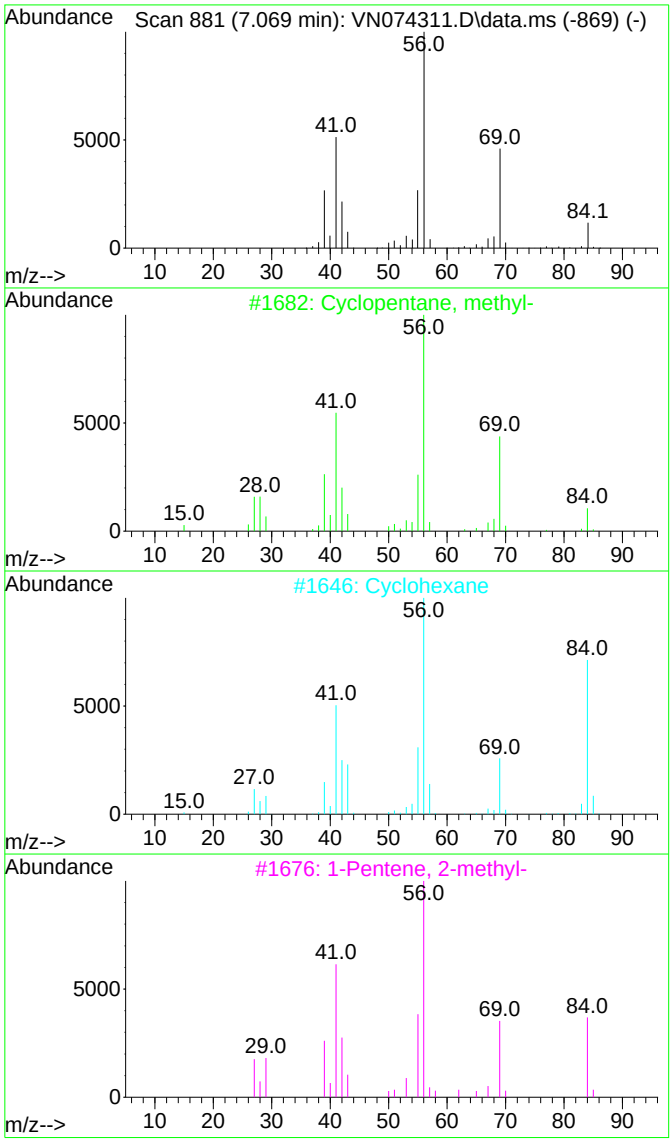
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090222W.M
Quant Title : SW846 8260

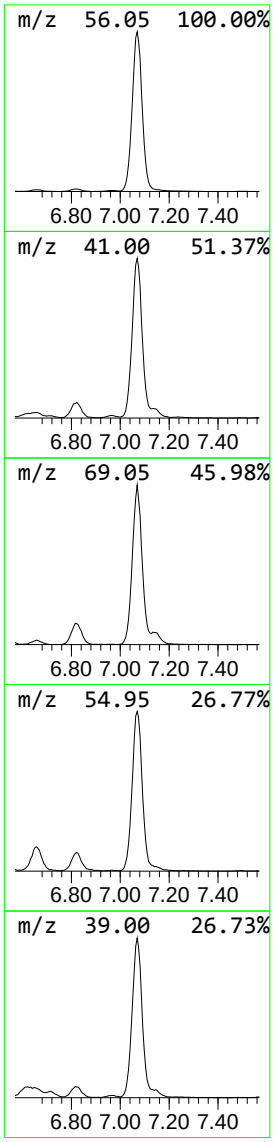
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.069	74.19 ug/l	26062600	Pentafluorobenzene	8.022

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2	Cyclohexane	84	C6H12	000110-82-7	78
3	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	72
4	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
5	Cyclobutane, ethyl-	84	C6H12	004806-61-5	72





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090222\
Data File : VN074311.D
Acq On : 03 Sep 2022 01:51
Operator : JC\MD
Sample : N4355-07
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 34 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP082322

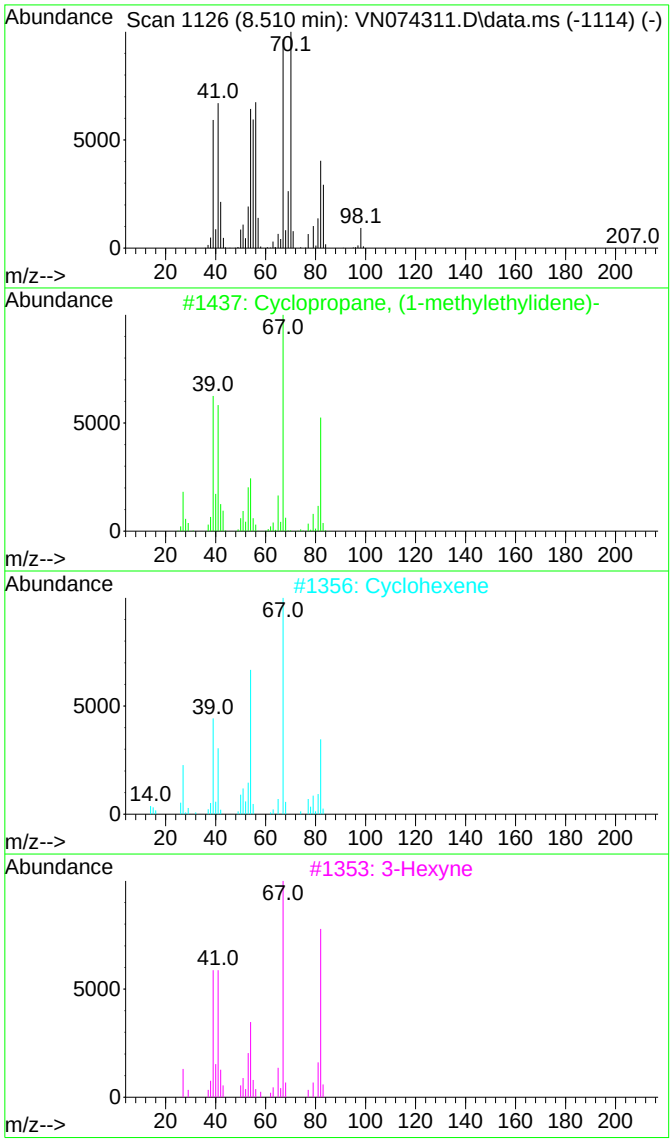
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090222W.M
Quant Title : SW846 8260

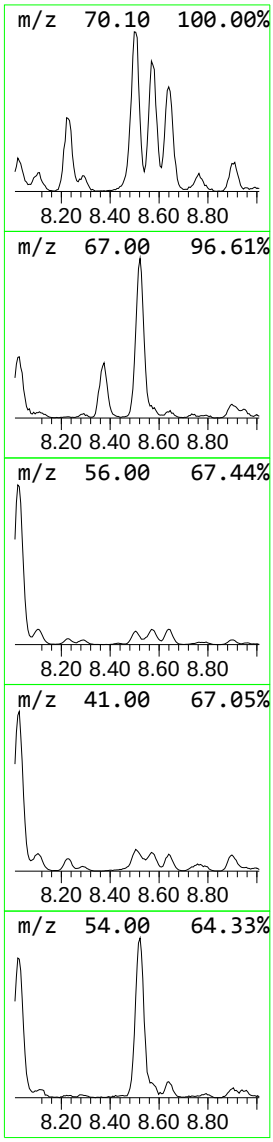
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Cyclopropane, (1-methylethy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.510	53.99 ug/l	4164090	1,4-Difluorobenzene	8.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropane, (1-methylethylidene)-	82	C6H10	004741-86-0	50
2	Cyclohexene	82	C6H10	000110-83-8	49
3	3-Hexyne	82	C6H10	000928-49-4	46
4	Cyclobutane, ethenyl-	82	C6H10	002597-49-1	46
5	Cyclopentane, 1,3-dimethyl-, cis-	98	C7H14	002532-58-3	46





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090222\
Data File : VN074311.D
Acq On : 03 Sep 2022 01:51
Operator : JC\MD
Sample : N4355-07
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 34 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP082322

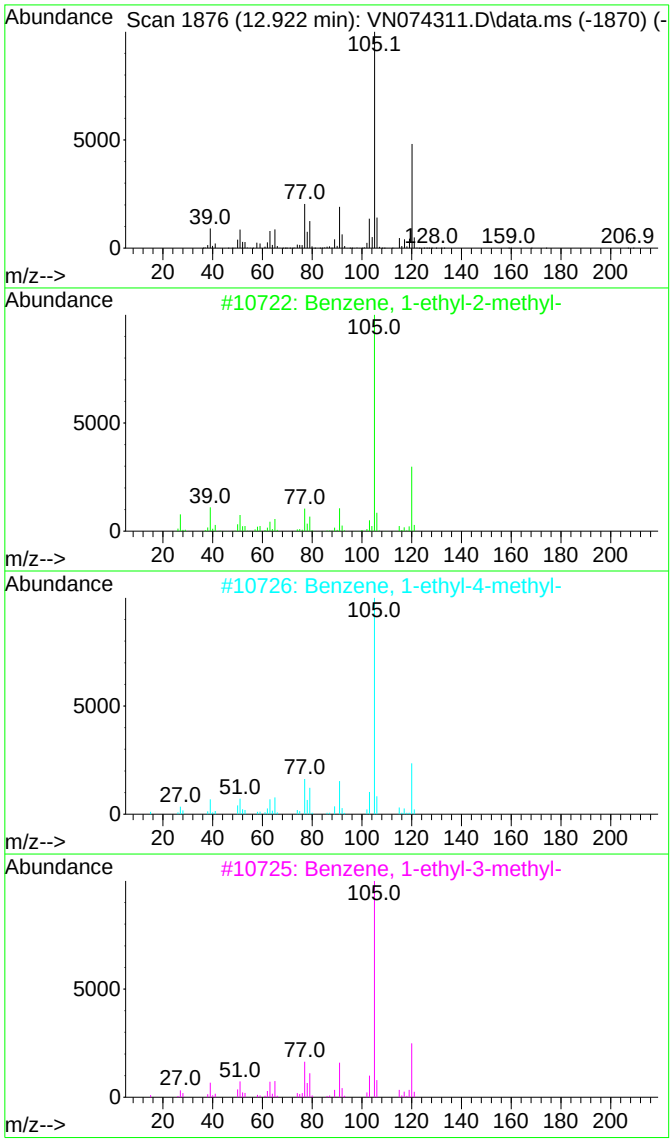
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090222W.M
Quant Title : SW846 8260

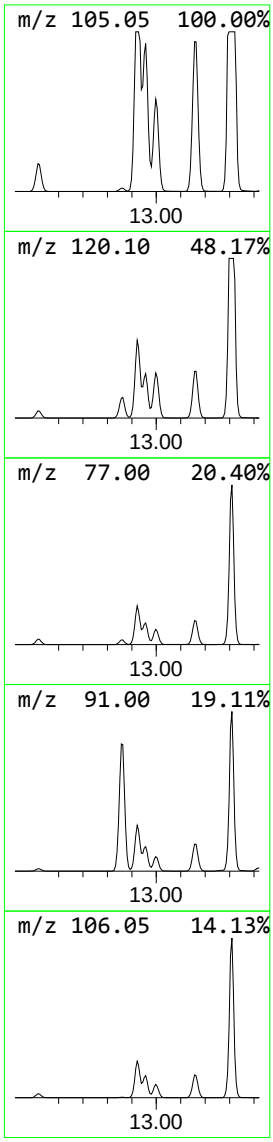
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, 1-ethyl-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.922	61.77 ug/l	50383100	1,4-Dichlorobenzene-d4	13.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	90
2	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90
3	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90
4	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	90
5	Mesitylene	120	C9H12	000108-67-8	87





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090222\
Data File : VN074311.D
Acq On : 03 Sep 2022 01:51
Operator : JC\MD
Sample : N4355-07
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 34 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP082322

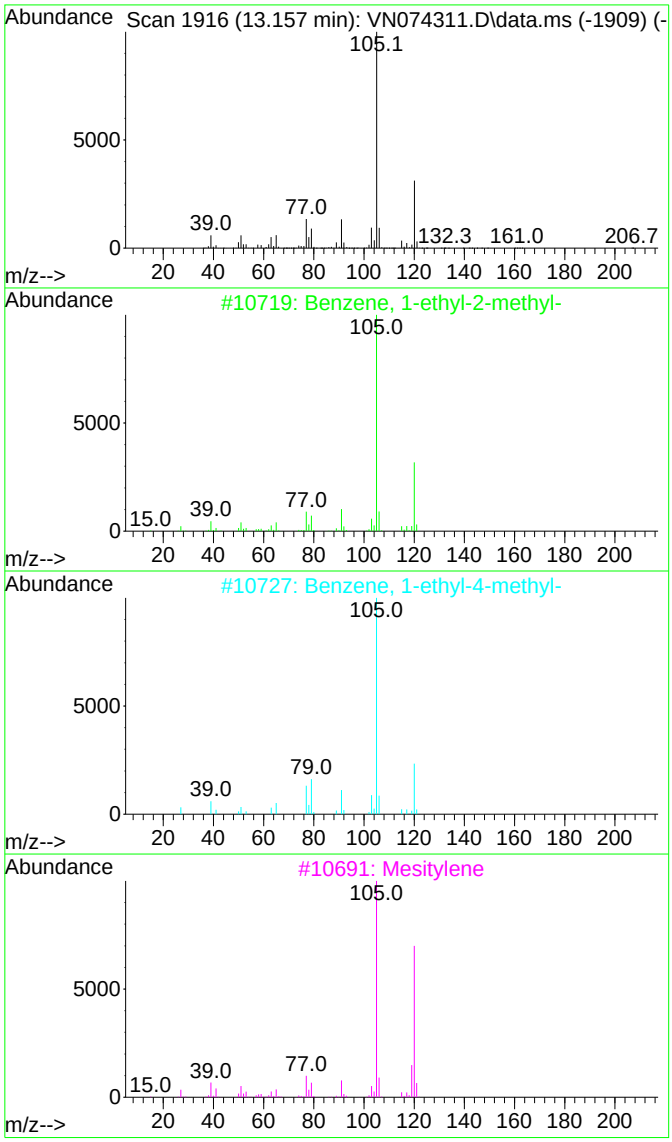
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090222W.M
Quant Title : SW846 8260

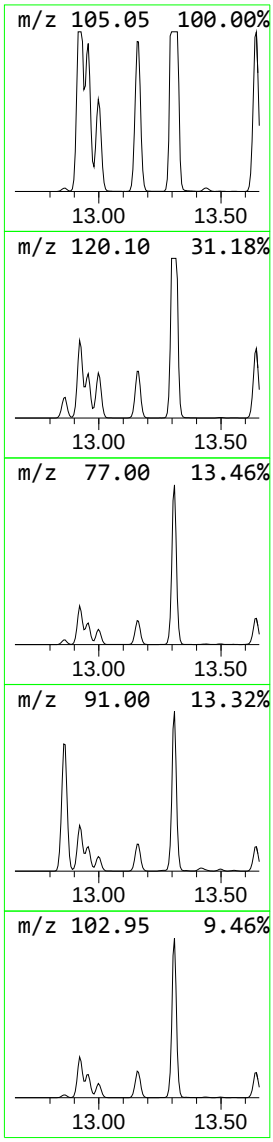
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, 1-ethyl-4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.157	40.39 ug/l	32947800	1,4-Dichlorobenzene-d4	13.610

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	93
3	Mesitylene	120	C9H12	000108-67-8	91
4	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090222\
Data File : VN074311.D
Acq On : 03 Sep 2022 01:51
Operator : JC\MD
Sample : N4355-07
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 34 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP082322

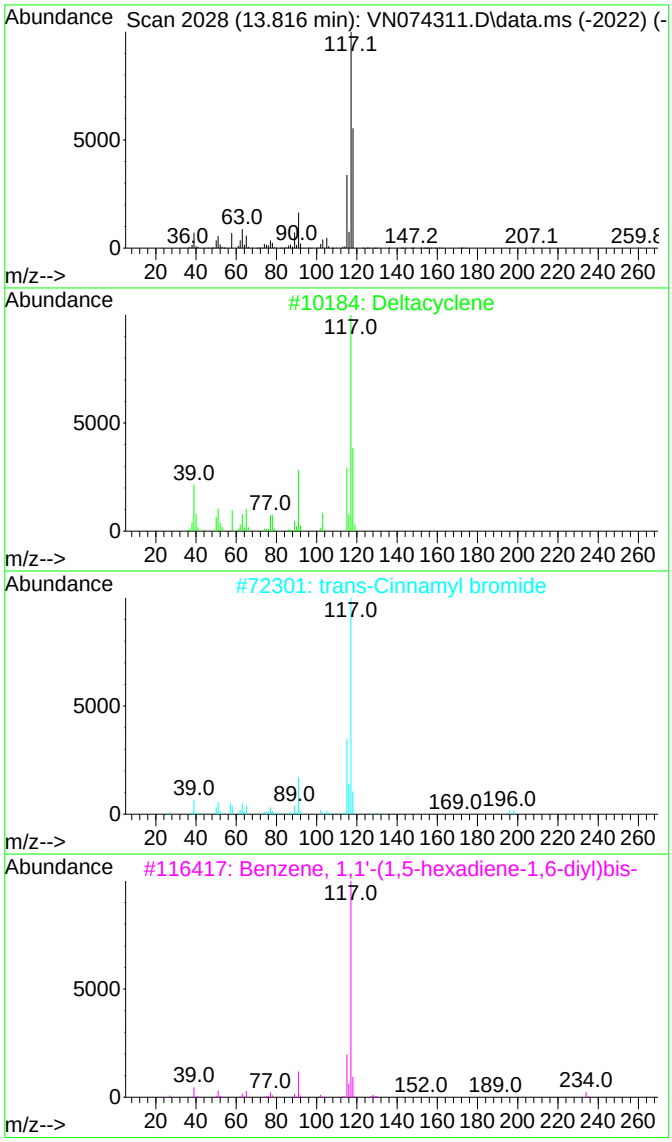
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090222W.M
Quant Title : SW846 8260

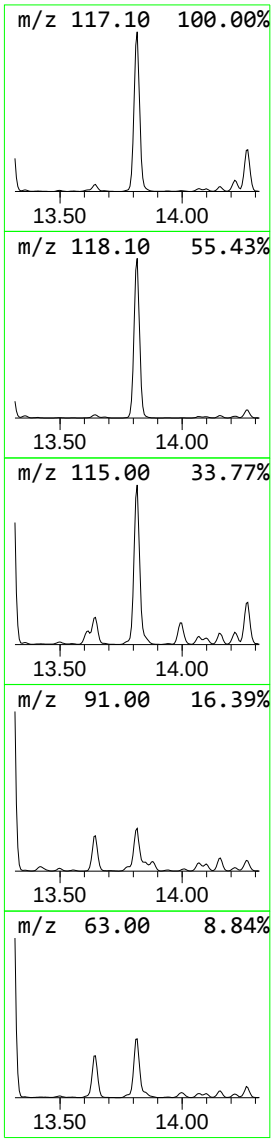
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 trans-Cinnamyl bromide Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.816	38.20 ug/l	31154900	1,4-Dichlorobenzene-d4	13.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Deltacyclene	118	C9H10	007785-10-6	59
2	trans-Cinnamyl bromide	196	C9H9Br	026146-77-0	53
3	Benzene, 1,1'-(1,5-hexadiene-1,6...	234	C18H18	004439-45-6	53
4	Indole	117	C8H7N	000120-72-9	49
5	Benzene, (2-bromocyclopropyl)-	196	C9H9Br	036617-02-4	45





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090222\
Data File : VN074311.D
Acq On : 03 Sep 2022 01:51
Operator : JC\MD
Sample : N4355-07
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 34 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP082322

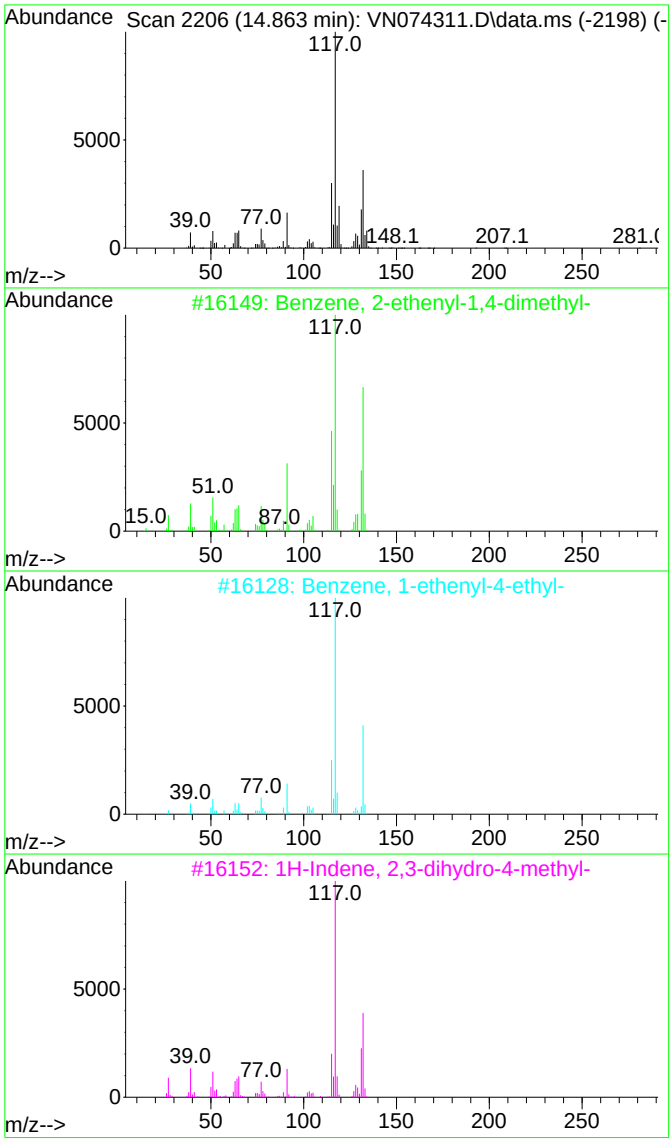
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090222W.M
Quant Title : SW846 8260

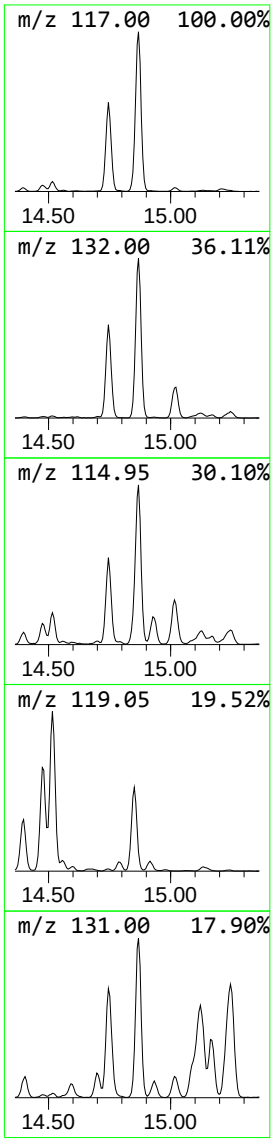
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.863	21.07 ug/l	17188800	1,4-Dichlorobenzene-d4	13.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	96
2	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
3	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	93
4	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	90
5	1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090222\
Data File : VN074311.D
Acq On : 03 Sep 2022 01:51
Operator : JC\MD
Sample : N4355-07
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 34 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DUP082322

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090222W.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
Butane, 2-methyl-	3.087	110.3	ug/l	38746800	1	8.022	17565600	50.0
Pentane	3.457	25.7	ug/l	9028750	1	8.022	17565600	50.0
unknown5.081	5.081	39.8	ug/l	13981800	1	8.022	17565600	50.0
Pentane, 3-methyl-	5.534	17.6	ug/l	6169880	1	8.022	17565600	50.0
Cyclopentane, m...	7.069	74.2	ug/l	26062600	1	8.022	17565600	50.0
Cyclopropane, (...	8.510	54.0	ug/l	4164090	2	8.904	3856130	50.0
Benzene, 1-ethy...	12.922	61.8	ug/l	50383100	4	13.610	40782300	50.0
Benzene, 1-ethy...	13.157	40.4	ug/l	32947800	4	13.610	40782300	50.0
trans-Cinnamyl ...	13.816	38.2	ug/l	31154900	4	13.610	40782300	50.0
Benzene, 2-ethe...	14.863	21.1	ug/l	17188800	4	13.610	40782300	50.0