

3Flex 5.02 3Flex Version 5.02 Page 1 of 22 Serial # 552 Unit 1 Port 3

Sample: DWTR-UT Fine

Operator: SMW Submitter: SMW

File: C:\3Flex\data\Sam Wallace\210914\_DWTRUT\_vialR\_port3.SMP

Started: 9/14/2021 2:25:18 PM Analysis adsorptive: N2

Completed: 9/15/2021 6:59:53 AM Analysis bath temp.: -195.911 °C

Report time: 9/15/2021 10:24:40 AM Thermal correction: No

Sample mass: 0.2357 g Ambient free space: 16.9393 cm<sup>3</sup> Measured

Analysis free space: 57.3371 cm³ Equilibration interval: 10 to 20 s Low pressure dose: 133.844 µmol/g Sample density: 1.000 g/cm³

Automatic degas: No

Comments: Micropore analysis, BET surface area, and pore volume

#### Summary Report

#### Surface Area

Single point surface area at  $p/p^{\circ} = 0.151442808$ : 194.0027 m<sup>2</sup>/g

BET Surface Area: 197.6077 m<sup>2</sup>/g

BJH Adsorption cumulative surface area of pores

between 15.000 Å and 1,000.000 Å diameter: 77.5506 m<sup>2</sup>/g

BJH Desorption cumulative surface area of pores

between 15.000 Å and 1,000.000 Å diameter: 157.3002 m<sup>2</sup>/g

#### Pore Volume

Single point adsorption total pore volume of pores

less than 2,597.391 Å diameter at p/p° = 0.992578361: 0.177007 cm<sup>3</sup>/g

Single point desorption total pore volume of pores

less than 3,173.700 Å diameter at p/p° = 0.993937967: 0.178124 cm³/g

BJH Adsorption cumulative volume of pores

between 15.000 Å and 1,000.000 Å diameter: 0.115867 cm³/g

BJH Desorption cumulative volume of pores

between 15.000 Å and 1,000.000 Å diameter: 0.156280 cm<sup>3</sup>/g

#### Pore Size

Adsorption average pore diameter (4V/A by BET): 35.830 Å

Desorption average pore diameter (4V/A by BET): 36.056 Å



3Flex 5.02 3Flex Version 5.02 Page 2 of 22 Serial # 552 Unit 1 Port 3

Sample: DWTR-UT Fine

Operator: SMW Submitter: SMW

File: C:\3Flex\data\Sam Wallace\210914\_DWTRUT\_vialR\_port3.SMP

Started: 9/14/2021 2:25:18 PM Analysis adsorptive: N2

Completed: 9/15/2021 6:59:53 AM Analysis bath temp.: -195.911 °C

Report time: 9/15/2021 10:24:40 AM Thermal correction: No

Sample mass: 0.2357 g Ambient free space: 16.9393 cm³ Measured

Analysis free space: 57.3371 cm³ Equilibration interval: 10 to 20 s
Low pressure dose: 133.844 µmol/g Sample density: 1.000 g/cm³

Automatic degas: No

Comments: Micropore analysis, BET surface area, and pore volume

Pore Size

BJH Adsorption average pore diameter (4V/A): 59.763 Å

BJH Desorption average pore diameter (4V/A): 39.740 Å



3Flex 5.02 3Flex Version 5.02 Page 3 of 22 Serial # 552 Unit 1 Port 3

Sample: DWTR-UT Fine

Operator: SMW Submitter: SMW

File: C:\3Flex\data\Sam Wallace\210914\_DWTRUT\_vialR\_port3.SMP

Started: 9/14/2021 2:25:18 PM Analysis adsorptive: N2

Completed: 9/15/2021 6:59:53 AM Analysis bath temp.: -195.911 °C

Report time: 9/15/2021 10:24:40 AM Thermal correction: No

Sample mass: 0.2357 g Ambient free space: 16.9393 cm³ Measured

Analysis free space: 57.3371 cm³ Equilibration interval: 10 to 20 s
Low pressure dose: 133.844 µmol/g Sample density: 1.000 g/cm³

Automatic degas: No

Comments: Micropore analysis, BET surface area, and pore volume

#### Isotherm Tabular Report

Relative Pressure (p/p°)	Absolute Pressure (mmHg)	Quantity Adsorbed (µmol/g)	Elapsed Time (h:min)	Saturation Pressure (mmHg)
			01:35	745.676025
0.000000668	0.000499	127.014	02:18	746.510742
0.000001909	0.001426	253.884	03:10	747.081482
0.000005585	0.004175	380.627	03:59	747.441345
0.000013947	0.010427	506.549	04:40	747.577209
0.000030733	0.022988	632.943	05:20	747.988037
0.000063170	0.047264	759.369	05:57	748.207397
0.000125666	0.094061	884.846	06:22	748.493774
0.000243920	0.182584	1009.815	07:06	748.539368
0.000480105	0.359641	1132.452	07:52	749.088318
0.000950013	0.712088	1250.575	08:54	749.555542
0.001860790	1.395188	1359.783	09:31	749.782410
0.003337649	2.501649	1457.140	10:24	749.524353
0.005497833	4.120709	1541.495	10:59	749.515076
0.008276560	6.203962	1612.984	11:19	749.582153
0.011474626	8.600367	1675.337	11:46	749.511719
0.021291943	15.957450	1794.656	11:57	749.459534
0.032818746	24.596066	1893.240	12:07	749.451721
0.039471795	29.583990	1939.698	12:13	749.496948
0.052977529	39.711010	2017.633	12:19	749.582153
0.116559137	87.378311	2256.174	12:26	749.647888
0.151442808	113.533615	2343.467	12:30	749.679810
0.203220089	152.351486	2442.216	12:35	749.687134
0.251333377	188.433472	2514.745	12:39	749.735168
0.301771740	226.244171	2578.666	12:43	749.719543
0.399114418	299.216644	2681.749	12:46	749.701416
0.499991126	374.828308	2782.132	12:50	749.669922
0.598562595	448.720245	2885.826	12:53	749.663025



3Flex 5.02 3Flex Version 5.02 Page 4 of 22 Serial # 552 Unit 1 Port 3

Sample: DWTR-UT Fine

Operator: SMW Submitter: SMW

File: C:\3Flex\data\Sam Wallace\210914\_DWTRUT\_vialR\_port3.SMP

Started: 9/14/2021 2:25:18 PM Analysis adsorptive: N2

Completed: 9/15/2021 6:59:53 AM Analysis bath temp.: -195.911 °C

Report time: 9/15/2021 10:24:40 AM Thermal correction: No

Sample mass: 0.2357 g Ambient free space: 16.9393 cm³ Measured

Analysis free space: 57.3371 cm³ Equilibration interval: 10 to 20 s
Low pressure dose: 133.844 µmol/g Sample density: 1.000 g/cm³

Automatic degas: No

Comments: Micropore analysis, BET surface area, and pore volume

#### Isotherm Tabular Report

Relative Pressure (p/p°)	Absolute Pressure (mmHg)	Quantity Adsorbed (µmol/g)	Elapsed Time (h:min)	Saturation Pressure (mmHg)
0.698666371	523.742981	3022.839	12:56	749.632446
0.718810003	538.874451	3059.359	12:59	749.675781
0.739801397	554.605591	3101.788	13:02	749.668213
0.758969965	569.071594	3146.482	13:05	749.794617
0.779899116	584.675049	3201.953	13:09	749.680359
0.799689451	599.574097	3264.696	13:11	749.758667
0.818967788	613.994507	3338.535	13:14	749.717529
0.838379323	628.612610	3433.240	13:18	749.794983
0.858102856	643.442749	3549.330	13:22	749.843384
0.879941182	659.779297	3724.755	13:29	749.799316
0.898509545	673.631592	3907.751	13:33	749.721130
0.910063760	682.385071	4032.096	13:37	749.821167
0.919631465	689.639404	4144.447	13:42	749.908447
0.929504685	697.071838	4264.790	13:46	749.939026
0.939240469	704.384949	4373.063	13:50	749.951660
0.949503563	712.096436	4488.404	13:54	749.967102
0.959706284	719.791077	4605.127	13:58	750.011841
0.969726812	727.273743	4716.343	14:01	749.977966
0.978881201	734.167114	4840.905	14:05	750.006348
0.987878439	740.925049	4985.477	14:09	750.016418
0.993937967	745.500916	5128.819	14:13	750.047729
0.991661106	743.714417	5106.729	14:16	749.968323
0.980283431	735.157349	4968.271	14:21	749.943665
0.969421288	727.071350	4869.907	14:25	750.005554
0.961156529	720.845398	4810.166	14:28	749.977112
0.950490370	712.836914	4743.586	14:31	749.967529
0.940133064	705.137268	4684.744	14:34	750.039856
0.930797479	698.132935	4633.511	14:37	750.037415



Page 5 of 22

3Flex 5.02 3Flex Version 5.02 Serial # 552 Unit 1 Port 3

Sample: DWTR-UT Fine

Operator: SMW Submitter: SMW

File: C:\3Flex\data\Sam Wallace\210914\_DWTRUT\_vialR\_port3.SMP

Started: 9/14/2021 2:25:18 PM Analysis adsorptive: N2

Completed: 9/15/2021 6:59:53 AM Analysis bath temp.: -195.911 °C

Report time: 9/15/2021 10:24:40 AM Thermal correction: No

Sample mass: 0.2357 g Ambient free space: 16.9393 cm³ Measured

Analysis free space: 57.3371 cm³ Equilibration interval: 10 to 20 s
Low pressure dose: 133.844 µmol/g Sample density: 1.000 g/cm³

Automatic degas: No

Comments: Micropore analysis, BET surface area, and pore volume

#### Isotherm Tabular Report

Relative Pressure (p/p°)	Absolute Pressure (mmHg)	Quantity Adsorbed (µmol/g)	Elapsed Time (h:min)	Saturation Pressure (mmHg)
0.920875089	690.727417	4582.148	14:41	750.077209
0.910505219	682.984558	4528.584	14:45	750.116028
0.900221453	675.213562	4471.130	14:50	750.052734
0.881085306	660.781982	4347.853	14:59	749.963684
0.862002076	646.573425	4205.459	15:04	750.083374
0.841878392	631.574097	4047.026	15:09	750.196350
0.821435659	616.190002	3887.852	15:14	750.137878
0.800369932	600.418823	3742.105	15:19	750.176636
0.780834597	585.834167	3627.575	15:23	750.266663
0.760925730	570.928650	3527.606	15:28	750.307983
0.740671081	555.755249	3444.672	15:32	750.340149
0.721142760	541.106812	3377.229	15:36	750.346313
0.700709205	525.856812	3317.339	15:40	750.463684
0.598715983	449.298889	3115.547	15:44	750.437439
0.501416305	376.287781	2991.278	15:48	750.449829
0.401380689	301.246643	2741.912	15:53	750.526001
0.295686295	221.942703	2623.152	15:58	750.601929
0.250557994	188.093109	2564.807	16:03	750.696899
0.200290404	150.344635	2489.976	16:07	750.633240
0.152543409	114.519516	2400.960	16:11	750.733948
0.100697864	75.597336	2267.773	16:16	750.734253
0.050548509	37.947880	2068.021	16:22	750.722046



3Flex 5.02 3Flex Version 5.02 Page 6 of 22 Serial # 552 Unit 1 Port 3

Sample: DWTR-UT Fine

Operator: SMW Submitter: SMW

File: C:\3Flex\data\Sam Wallace\210914\_DWTRUT\_vialR\_port3.SMP

Started: 9/14/2021 2:25:18 PM Analysis adsorptive: N2

Completed: 9/15/2021 6:59:53 AM Analysis bath temp.: -195.911 °C

Report time: 9/15/2021 10:24:40 AM Thermal correction: No

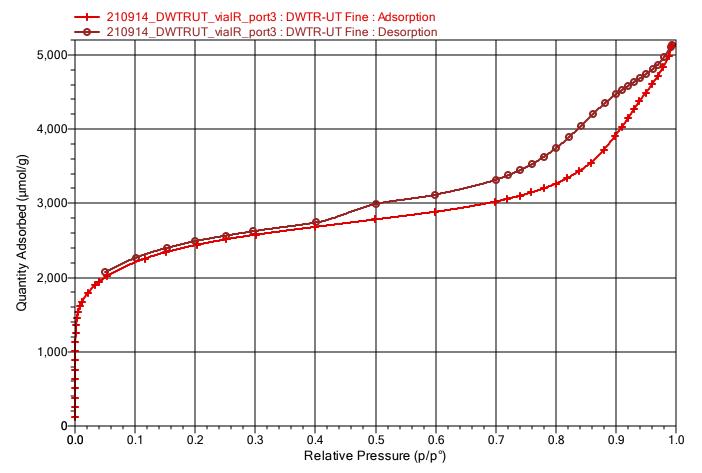
Sample mass: 0.2357 g Ambient free space: 16.9393 cm³ Measured

Analysis free space: 57.3371 cm³ Equilibration interval: 10 to 20 s
Low pressure dose: 133.844 µmol/g Sample density: 1.000 g/cm³

Automatic degas: No

Comments: Micropore analysis, BET surface area, and pore volume

#### Isotherm Linear Plot





3Flex 5.02 3Flex Version 5.02 Page 7 of 22 Serial # 552 Unit 1 Port 3

Sample: DWTR-UT Fine

Operator: SMW Submitter: SMW

File: C:\3Flex\data\Sam Wallace\210914\_DWTRUT\_vialR\_port3.SMP

Started: 9/14/2021 2:25:18 PM Analysis adsorptive: N2

Completed: 9/15/2021 6:59:53 AM Analysis bath temp.: -195.911 °C

Report time: 9/15/2021 10:24:40 AM Thermal correction: No

Sample mass: 0.2357 g Ambient free space: 16.9393 cm³ Measured

Analysis free space: 57.3371 cm³ Equilibration interval: 10 to 20 s
Low pressure dose: 133.844 µmol/g Sample density: 1.000 g/cm³

Automatic degas: No

Comments: Micropore analysis, BET surface area, and pore volume

#### **BET Report**

BET surface area:  $197.6077 \pm 0.8856 \text{ m}^2/\text{g}$ 

Slope:  $0.0004922 \pm 0.0000022 \text{ g/}\mu\text{mol}$  Y-intercept:  $0.0000015 \pm 0.0000002 \text{ g/}\mu\text{mol}$ 

C: 331.308273 Qm: 2,025.517 µmol/g

Correlation coefficient: 0.9999397 Molecular cross-sectional area: 0.1620 nm²

Relative Pressure (p/p°)	Quantity Adsorbed (μmol/g)	1/[Q(p°/p - 1)]
0.008276560	1612.984	0.0000052
0.011474626	1675.337	0.0000069
0.021291943	1794.656	0.0000121
0.032818746	1893.240	0.0000179
0.039471795	1939.698	0.0000212
0.052977529	2017.633	0.0000277
0.116559137	2256.174	0.0000585
0.151442808	2343.467	0.0000762



3Flex 5.02 3Flex Version 5.02 Page 8 of 22 Serial # 552 Unit 1 Port 3

Sample: DWTR-UT Fine

Operator: SMW Submitter: SMW

File: C:\3Flex\data\Sam Wallace\210914\_DWTRUT\_vialR\_port3.SMP

Started: 9/14/2021 2:25:18 PM Analysis adsorptive: N2

Completed: 9/15/2021 6:59:53 AM Analysis bath temp.: -195.911 °C

Report time: 9/15/2021 10:24:40 AM Thermal correction: No

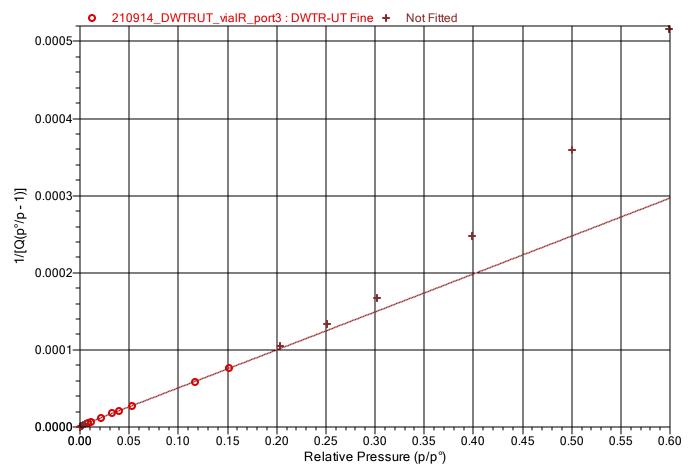
Sample mass: 0.2357 g Ambient free space: 16.9393 cm³ Measured

Analysis free space: 57.3371 cm³ Equilibration interval: 10 to 20 s
Low pressure dose: 133.844 µmol/g Sample density: 1.000 g/cm³

Automatic degas: No

Comments: Micropore analysis, BET surface area, and pore volume

#### **BET Surface Area Plot**





3Flex 5.02 3Flex Version 5.02 Page 9 of 22 Serial # 552 Unit 1 Port 3

Sample: DWTR-UT Fine

Operator: SMW Submitter: SMW

File: C:\3Flex\data\Sam Wallace\210914\_DWTRUT\_vialR\_port3.SMP

Started: 9/14/2021 2:25:18 PM Analysis adsorptive: N2

Completed: 9/15/2021 6:59:53 AM Analysis bath temp.: -195.911 °C

Report time: 9/15/2021 10:24:40 AM Thermal correction: No

Sample mass: 0.2357 g Ambient free space: 16.9393 cm³ Measured

Analysis free space: 57.3371 cm³ Equilibration interval: 10 to 20 s
Low pressure dose: 133.844 µmol/g Sample density: 1.000 g/cm³

Automatic degas: No

Comments: Micropore analysis, BET surface area, and pore volume

#### BJH Desorption Pore Distribution Report

Standard Halsey  $t = 3.54 [-5 / ln(p/p^{\circ})]^{0.333}$ 

Diameter range: 15.000 to 1,000.000 Å

Adsorbate property factor: 9.53000 Å

Density conversion factor: 0.0015495

Fraction of pores open at both ends: 0.00

Pore Diameter Range (Å)	Average Diameter (Å)	Incremental Pore Volume (cm³/g)	Cumulative Pore Volume (cm³/g)	Incremental Pore Area (m²/g)	Cumulative Pore Area (m²/g)
1001.7 - 652.2	754.2	0.003753	0.003753	0.199	0.199
652.2 - 516.6	568.2	0.002308	0.006061	0.162	0.361
516.6 - 408.0	449.1	0.002618	0.008678	0.233	0.595
408.0 - 339.3	367.1	0.002353	0.011031	0.256	0.851
339.3 - 294.9	313.8	0.002083	0.013114	0.265	1.116
294.9 - 259.0	274.5	0.002118	0.015232	0.309	1.425
259.0 - 229.9	242.6	0.002247	0.017480	0.370	1.796
229.9 - 206.9	217.1	0.002459	0.019938	0.453	2.249
206.9 - 174.6	187.8	0.005449	0.025387	1.160	3.409
174.6 - 151.2	161.1	0.006488	0.031875	1.611	5.020
151.2 - 132.5	140.5	0.007403	0.039278	2.108	7.128
132.5 - 117.7	124.1	0.007596	0.046875	2.448	9.576
117.7 - 105.5	110.9	0.007049	0.053924	2.543	12.119
105.5 - 96.3	100.4	0.005569	0.059493	2.218	14.337
96.3 - 88.4	92.0	0.004880	0.064373	2.123	16.460
88.4 - 81.6	84.7	0.004021	0.068394	1.900	18.359
81.6 - 75.9	78.5	0.003245	0.071640	1.654	20.014
75.9 - 70.7	73.0	0.002851	0.074491	1.561	21.575
70.7 - 52.3	58.3	0.009745	0.084236	6.686	28.262



3Flex 5.02 3Flex Version 5.02 Page 10 of 22 Serial # 552 Unit 1 Port 3

Sample: DWTR-UT Fine

Operator: SMW Submitter: SMW

File: C:\3Flex\data\Sam Wallace\210914\_DWTRUT\_vialR\_port3.SMP

Started: 9/14/2021 2:25:18 PM Analysis adsorptive: N2

Completed: 9/15/2021 6:59:53 AM Analysis bath temp.: -195.911 °C

Report time: 9/15/2021 10:24:40 AM Thermal correction: No

Sample mass: 0.2357 g Ambient free space: 16.9393 cm³ Measured

Analysis free space: 57.3371 cm³ Equilibration interval: 10 to 20 s
Low pressure dose: 133.844 µmol/g Sample density: 1.000 g/cm³

Automatic degas: No

Comments: Micropore analysis, BET surface area, and pore volume

Pore Diameter Range (Å)	Average Diameter (Å)	Incremental Pore Volume (cm³/g)	Cumulative Pore Volume (cm³/g)	Incremental Pore Area (m²/g)	Cumulative Pore Area (m²/g)
52.3 - 41.3	45.2	0.005546	0.089781	4.904	33.166
41.3 - 33.4	36.3	0.016830	0.106611	18.560	51.726
33.4 - 27.0	29.3	0.004991	0.111602	6.816	58.542
27.0 - 24.6	25.7	0.002928	0.114531	4.565	63.107
24.6 - 22.2	23.2	0.004369	0.118900	7.523	70.630
22.2 - 19.9	20.9	0.006192	0.125092	11.853	82.484
19.9 - 17.5	18.5	0.011224	0.136317	24.298	106.782
17.5 - 14.8	15.8	0.019963	0.156280	50.518	157.300



3Flex 5.02 3Flex Version 5.02 Page 11 of 22 Serial #552 Unit 1 Port 3

Sample: DWTR-UT Fine

Operator: SMW Submitter: SMW

File: C:\3Flex\data\Sam Wallace\210914\_DWTRUT\_vialR\_port3.SMP

Started: 9/14/2021 2:25:18 PM Analysis adsorptive: N2 Completed: 9/15/2021 6:59:53 AM Analysis bath temp.: -195.911 °C

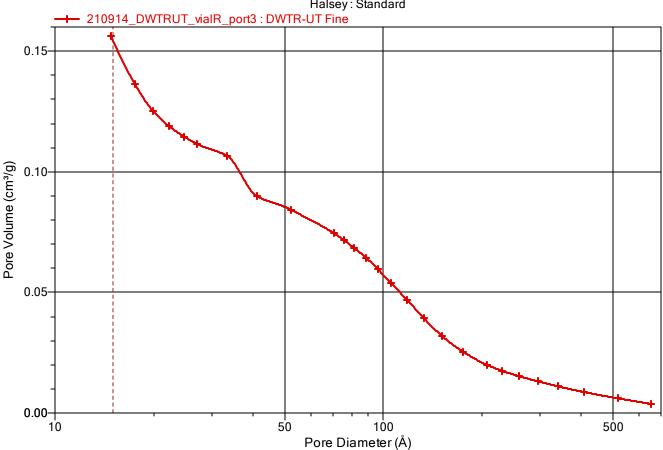
Report time: 9/15/2021 10:24:40 AM Thermal correction: No

Sample mass: 0.2357 g Ambient free space: 16.9393 cm<sup>3</sup> Measured Analysis free space: 57.3371 cm<sup>3</sup> Equilibration interval: 10 to 20 s Low pressure dose: 133.844 µmol/g Sample density: 1.000 g/cm<sup>3</sup>

Automatic degas: No

Comments: Micropore analysis, BET surface area, and pore volume

### BJH Desorption Cumulative Pore Volume (Larger)





3Flex 5.02 3Flex Version 5.02 Page 12 of 22 Serial #552 Unit 1 Port 3

Sample: DWTR-UT Fine

Operator: SMW Submitter: SMW

File: C:\3Flex\data\Sam Wallace\210914\_DWTRUT\_vialR\_port3.SMP

Started: 9/14/2021 2:25:18 PM Analysis adsorptive: N2

Completed: 9/15/2021 6:59:53 AM Analysis bath temp.: -195.911 °C

Report time: 9/15/2021 10:24:40 AM Thermal correction: No

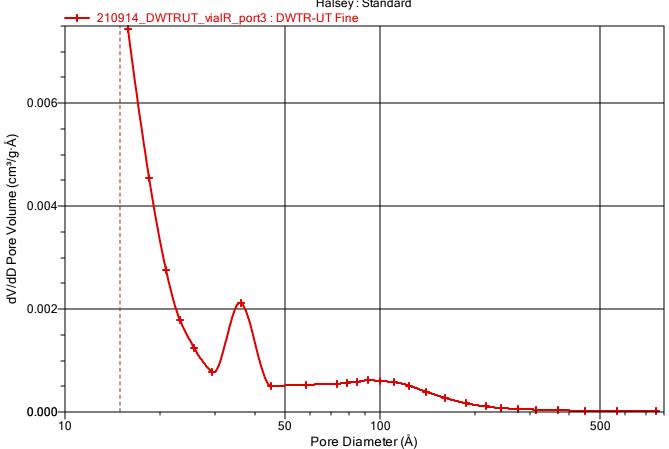
Sample mass: 0.2357 g Ambient free space: 16.9393 cm<sup>3</sup> Measured

Analysis free space: 57.3371 cm<sup>3</sup> Equilibration interval: 10 to 20 s Low pressure dose: 133.844 µmol/g Sample density: 1.000 g/cm<sup>3</sup>

Automatic degas: No

Comments: Micropore analysis, BET surface area, and pore volume

### BJH Desorption dV/dD Pore Volume





3Flex 5.02 3Flex Version 5.02 Page 13 of 22 Serial #552 Unit 1 Port 3

Sample: DWTR-UT Fine

Operator: SMW Submitter: SMW

File: C:\3Flex\data\Sam Wallace\210914\_DWTRUT\_vialR\_port3.SMP

Started: 9/14/2021 2:25:18 PM Analysis adsorptive: N2

Completed: 9/15/2021 6:59:53 AM Analysis bath temp.: -195.911 °C

Report time: 9/15/2021 10:24:40 AM Thermal correction: No

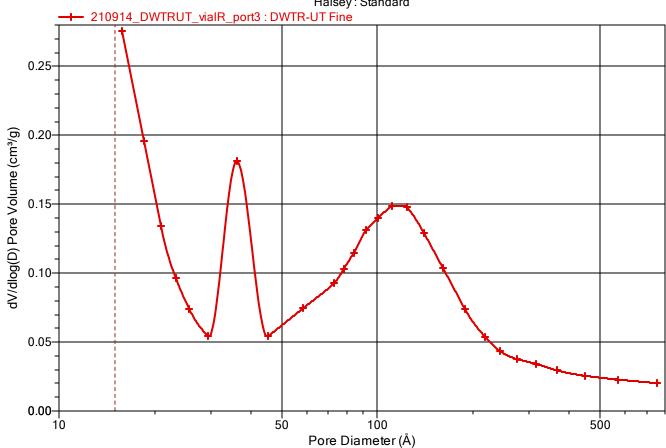
Sample mass: 0.2357 g Ambient free space: 16.9393 cm<sup>3</sup> Measured

Analysis free space: 57.3371 cm<sup>3</sup> Equilibration interval: 10 to 20 s Low pressure dose: 133.844 µmol/g Sample density: 1.000 g/cm<sup>3</sup>

Automatic degas: No

Comments: Micropore analysis, BET surface area, and pore volume

### BJH Desorption dV/dlog(D) Pore Volume





3Flex 5.02 3Flex Version 5.02 Page 14 of 22 Serial # 552 Unit 1 Port 3

Sample: DWTR-UT Fine

Operator: SMW Submitter: SMW

File: C:\3Flex\data\Sam Wallace\210914\_DWTRUT\_vialR\_port3.SMP

Started: 9/14/2021 2:25:18 PM Analysis adsorptive: N2

Completed: 9/15/2021 6:59:53 AM Analysis bath temp.: -195.911 °C

Report time: 9/15/2021 10:24:40 AM Thermal correction: No

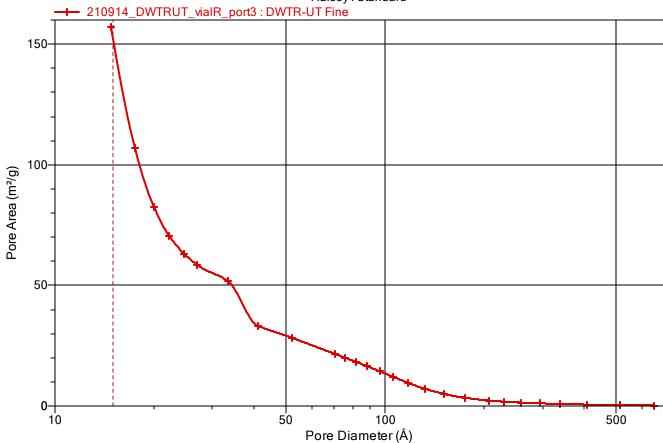
Sample mass: 0.2357 g Ambient free space: 16.9393 cm³ Measured

Analysis free space: 57.3371 cm³ Equilibration interval: 10 to 20 s
Low pressure dose: 133.844 µmol/g Sample density: 1.000 g/cm³

Automatic degas: No

Comments: Micropore analysis, BET surface area, and pore volume

### BJH Desorption Cumulative Pore Area (Larger)





3Flex 5.02 3Flex Version 5.02 Page 15 of 22 Serial #552 Unit 1 Port 3

Sample: DWTR-UT Fine

Operator: SMW Submitter: SMW

File: C:\3Flex\data\Sam Wallace\210914\_DWTRUT\_vialR\_port3.SMP

Started: 9/14/2021 2:25:18 PM Analysis adsorptive: N2

Completed: 9/15/2021 6:59:53 AM Analysis bath temp.: -195.911 °C

Report time: 9/15/2021 10:24:40 AM Thermal correction: No

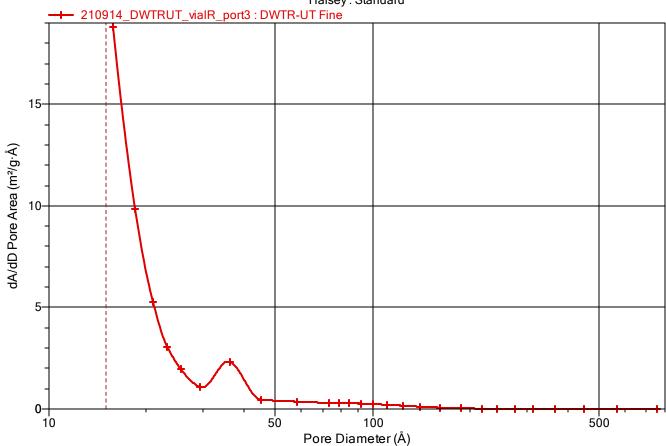
Sample mass: 0.2357 g Ambient free space: 16.9393 cm<sup>3</sup> Measured

Analysis free space: 57.3371 cm<sup>3</sup> Equilibration interval: 10 to 20 s Low pressure dose: 133.844 µmol/g Sample density: 1.000 g/cm<sup>3</sup>

Automatic degas: No

Comments: Micropore analysis, BET surface area, and pore volume

### BJH Desorption dA/dD Pore Area





3Flex 5.02 3Flex Version 5.02 Page 16 of 22 Serial #552 Unit 1 Port 3

Sample: DWTR-UT Fine

Operator: SMW Submitter: SMW

File: C:\3Flex\data\Sam Wallace\210914\_DWTRUT\_vialR\_port3.SMP

Started: 9/14/2021 2:25:18 PM Analysis adsorptive: N2

Completed: 9/15/2021 6:59:53 AM Analysis bath temp.: -195.911 °C

Report time: 9/15/2021 10:24:40 AM Thermal correction: No

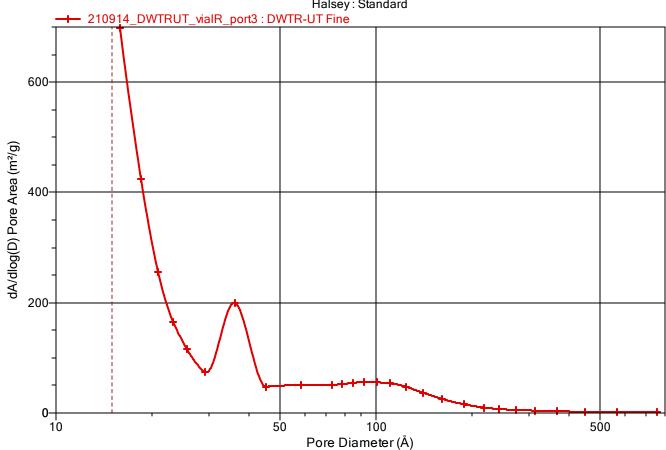
Sample mass: 0.2357 g Ambient free space: 16.9393 cm<sup>3</sup> Measured

Analysis free space: 57.3371 cm<sup>3</sup> Equilibration interval: 10 to 20 s Low pressure dose: 133.844 µmol/g Sample density: 1.000 g/cm<sup>3</sup>

Automatic degas: No

Comments: Micropore analysis, BET surface area, and pore volume

### BJH Desorption dA/dlog(D) Pore Area





3Flex Version 5.02 Serial # 552 Unit 1 Port 3 Page 17 of 22

Sample: DWTR-UT Fine

Operator: SMW Submitter: SMW

File: C:\3Flex\data\Sam Wallace\210914\_DWTRUT\_vialR\_port3.SMP

Started: 9/14/2021 2:25:18 PM Analysis adsorptive: N2

Completed: 9/15/2021 6:59:53 AM Analysis bath temp.: -195.911 °C

Report time: 9/15/2021 10:24:40 AM Thermal correction: No

Sample mass: 0.2357 g Ambient free space: 16.9393 cm³ Measured

Analysis free space: 57.3371 cm³ Equilibration interval: 10 to 20 s
Low pressure dose: 133.844 µmol/g Sample density: 1.000 g/cm³

Automatic degas: No

3Flex 5.02

Comments: Micropore analysis, BET surface area, and pore volume

# Horvath-Kawazoe Report Cylinder Pore Geometry (Saito-Foley)

Maximum pore volume: 0.067366 cm³/g at Relative Pressure: 0.039471795 Median pore width: 11.532 Å

Relative pressure range: 1e-09 to 0.0406159

Diameter of adsorptive molecule: 3.000 Å

Adsorptive density: 6.710e+14 molecules/cm<sup>2</sup>

Adsorptive dispersion constant: 7.777e-59 Diameter of sample atom: 3.040 Å

Sample Density: 3.750e+15 molecules/cm<sup>2</sup>

Sample dispersion constant: 7.923e-59

Density conversion factor: 0.0015495

Absolute Pressure (mmHg)	Relative Pressure (p/p°)	Quantity Adsorbed (μmol/g)	Pore Width (Å)	Cumulative Pore Volume (cm³/g)	Differential Pore Volume (cm³/g·Å)
0.00050	0.000000668	127.01429	7.933	0.0044	0.0006
0.00143	0.000001909	253.88412	8.378	0.0088	0.0099
0.00417	0.000005585	380.62738	8.904	0.0132	0.0084
0.01043	0.000013947	506.54851	9.426	0.0176	0.0084
0.02299	0.000030733	632.94335	9.945	0.0220	0.0085
0.04726	0.000063170	759.36850	10.486	0.0264	0.0081
0.09406	0.000125666	884.84580	11.079	0.0307	0.0074
0.18258	0.000243920	1009.81451	11.738	0.0351	0.0066
0.35964	0.000480105	1132.45181	12.521	0.0393	0.0054
0.71209	0.000950013	1250.57544	13.458	0.0434	0.0044
1.39519	0.001860790	1359.78343	14.570	0.0472	0.0034
2.50165	0.003337649	1457.13999	15.741	0.0506	0.0029



3Flex 5.02 3Flex Version 5.02 Page 18 of 22 Serial # 552 Unit 1 Port 3

Sample: DWTR-UT Fine

Operator: SMW Submitter: SMW

File: C:\3Flex\data\Sam Wallace\210914\_DWTRUT\_vialR\_port3.SMP

Started: 9/14/2021 2:25:18 PM Analysis adsorptive: N2

Completed: 9/15/2021 6:59:53 AM Analysis bath temp.: -195.911 °C

Report time: 9/15/2021 10:24:40 AM Thermal correction: No

Sample mass: 0.2357 g Ambient free space: 16.9393 cm³ Measured

Analysis free space: 57.3371 cm³ Equilibration interval: 10 to 20 s
Low pressure dose: 133.844 µmol/g Sample density: 1.000 g/cm³

Automatic degas: No

Comments: Micropore analysis, BET surface area, and pore volume

Absolute Pressure (mmHg)	Relative Pressure (p/p°)	Quantity Adsorbed (µmol/g)	Pore Width (Å)	Cumulative Pore Volume (cm³/g)	Differential Pore Volume (cm³/g·Å)
4.12071	0.005497833	1541.49538	16.943	0.0535	0.0024
6.20396	0.008276560	1612.98417	18.108	0.0560	0.0021
8.60037	0.011474626	1675.33658	19.187	0.0582	0.0020
15.95745	0.021291943	1794.65631	21.721	0.0623	0.0016
24.59607	0.032818746	1893.24009	24.023	0.0658	0.0015
29.58399	0.039471795	1939.69800	25.201	0.0674	0.0014



3Flex 5.02 3Flex Version 5.02 Page 19 of 22 Serial # 552 Unit 1 Port 3

Sample: DWTR-UT Fine

Operator: SMW Submitter: SMW

File: C:\3Flex\data\Sam Wallace\210914\_DWTRUT\_vialR\_port3.SMP

Started: 9/14/2021 2:25:18 PM Analysis adsorptive: N2

Completed: 9/15/2021 6:59:53 AM Analysis bath temp.: -195.911 °C

Report time: 9/15/2021 10:24:40 AM Thermal correction: No

Sample mass: 0.2357 g Ambient free space: 16.9393 cm³ Measured

Analysis free space: 57.3371 cm³ Equilibration interval: 10 to 20 s Low pressure dose: 133.844 µmol/g Sample density: 1.000 g/cm³

Automatic degas: No

Comments: Micropore analysis, BET surface area, and pore volume

# Sample Information

Method: Catalyst & Catalyst Carrier Pore Size - ASTM D4222

Sample: DWTR-UT Fine

Operator: SMW
Submitter: SMW
Mass type: Calculated
Empty tube: 46.3864 g
Sample + tube: 46.6221 g
Sample mass: 0.2357 g
Density: 1.000 g/cm³

Type of data: Automatically collected

Instrument type: 3500 Original instrument type: 3500

Comments: Micropore analysis, BET surface area, and pore volume

# Sample Tube

Sample tube: Sample Tube Ambient free space: 1.0000 cm³ Analysis free space: 1.0000 cm³ Use isothermal jacket: No

Use filler rod: No Vacuum seal type: None

### **Degas Conditions**

Degas conditions: According to ASTM Test Method D4222

Smart VacPrep evacuation

Backfill sample tube: No

Evacuation rate: 5.0 mmHg/s



3Flex 5.02 3Flex Version 5.02 Page 20 of 22 Serial # 552 Unit 1 Port 3

Sample: DWTR-UT Fine

Operator: SMW Submitter: SMW

File: C:\3Flex\data\Sam Wallace\210914\_DWTRUT\_vialR\_port3.SMP

Started: 9/14/2021 2:25:18 PM Analysis adsorptive: N2

Completed: 9/15/2021 6:59:53 AM Analysis bath temp.: -195.911 °C

Report time: 9/15/2021 10:24:40 AM Thermal correction: No

Sample mass: 0.2357 g Ambient free space: 16.9393 cm³ Measured

Analysis free space: 57.3371 cm³ Equilibration interval: 10 to 20 s
Low pressure dose: 133.844 µmol/g Sample density: 1.000 g/cm³

Automatic degas: No

Comments: Micropore analysis, BET surface area, and pore volume

#### Smart VacPrep evacuation

Unrest. evacuation from: 5.0 mmHg

Vacuum level: 1.000000e-02 mmHg

Evacuation time: 10 min
Temperature ramp rate: 10.0 °C/min
Target temperature: 30 °C
Hold pressure: 100 mmHg

#### **Heating Phase**

Sample prep: Stage			Time (min)
1	30	10	10

# **Analysis Conditions**

Analysis conditions: According to ASTM Test Method D4222-03

Absolute pressure dosing: No Set external trigger: No

#### Pressure Table

Starting Pressure (p/p°)	Pressure Increment (p/p°)	Dose Amount (μmol/g)	Equilibration Interval (s)	Ending Pressure (p/p°)
0.000000000		133.844	20	0.010000000
0.010000000	0.010000000		15	0.050000000
0.050000000	0.050000000		15	0.300000000
0.300000000	0.100000000		10	0.700000000
0.70000000	0.020000000		10	0.900000000
0.90000000	0.010000000		10	0.990000000
0.990000000			10	0.995000000
0.995000000			10	0.990000000
0.990000000	0.010000000		10	0.900000000



3Flex 5.02 3Flex Version 5.02 Page 21 of 22 Serial # 552 Unit 1 Port 3

Sample: DWTR-UT Fine

Operator: SMW Submitter: SMW

File: C:\3Flex\data\Sam Wallace\210914\_DWTRUT\_vialR\_port3.SMP

Started: 9/14/2021 2:25:18 PM Analysis adsorptive: N2

Completed: 9/15/2021 6:59:53 AM Analysis bath temp.: -195.911 °C

Report time: 9/15/2021 10:24:40 AM Thermal correction: No

Sample mass: 0.2357 g Ambient free space: 16.9393 cm³ Measured

Analysis free space: 57.3371 cm³ Equilibration interval: 10 to 20 s
Low pressure dose: 133.844 µmol/g Sample density: 1.000 g/cm³

Automatic degas: No

Comments: Micropore analysis, BET surface area, and pore volume

#### Pressure Table

Starting Pressure (p/p°)	Pressure Increment (p/p°)	Dose Amount (μmol/g)	Equilibration Interval (s)	Ending Pressure (p/p°)
0.900000000	0.020000000		15	0.70000000
0.700000000	0.100000000		15	0.300000000
0.300000000	0.050000000		15	0.050000000

#### Preparation

Match transducer: Yes

Backfill gas: Nitrogen

Evacuation rate: 5.0 mmHg/s Unrestricted evacuation from: 5.0 mmHg

Vacuum level: 1.0e-03 mmHg

Evacuation time: 0.10 h

Degas in situ: No

Leak test: No

Elevator operation: Automatic

Free Space

Measured before analysis

Lower Dewar for evacuation: Yes

Evacuation time: 0.50 h

Outgas test: Yes

Outgas test duration: 120 s

p° and Temperature

p° type: Measured in Psat tube for each point

Temperature type: Calculated from p° or Psat



3Flex 5.02 3Flex Version 5.02 Page 22 of 22 Serial #552 Unit 1 Port 3

Sample: DWTR-UT Fine

Operator: SMW Submitter: SMW

File: C:\3Flex\data\Sam Wallace\210914\_DWTRUT\_vialR\_port3.SMP

Started: 9/14/2021 2:25:18 PM Analysis adsorptive: N2

Completed: 9/15/2021 6:59:53 AM Analysis bath temp.: -195.911 °C

Thermal correction: No Report time: 9/15/2021 10:24:40 AM

Sample mass: 0.2357 g Ambient free space: 16.9393 cm3 Measured

Analysis free space: 57.3371 cm<sup>3</sup> Equilibration interval: 10 to 20 s Low pressure dose: 133.844 µmol/g Sample density: 1.000 g/cm<sup>3</sup>

Automatic degas: No

Comments: Micropore analysis, BET surface area, and pore volume

#### Dosing

Target tolerance: 2.0% or 2.000 mmHg

Minimum equilibration delay at p/p $^{\circ}$  >= 0.995: 600 s

Minimum equilibration delay: 0.00 h Maximum equilibration delay: 999.00 h

#### Termination

Backfill at end of analysis: Yes

Backfill gas: Nitrogen

### Adsorptive Properties

Adsorptive: Nitrogen (N2)

Maximum manifold pressure: 925.00 mmHg

Therm. tran. hard-sphere diameter: 3.6810 Å

Molecular cross-sectional area: 0.162 nm²

Adsorbate molecular weight: 28.01

Mass flow constant: 1.000

Thermal conductivity: 1.00

Gas blend: No

Adsorbed-phase free-space correction: Yes

Fluid properties: H:\3500\files\fpi\nitrogen.fpi

Dosing method: Normal