## BWIQ Prediction Results Report

## Chemometrics model information:

Model file: Predict\_Using\_Model\_1

Joint\_x-y\_distances\_samples\_partition nSamples="21"

airPLS\_Baseline-Correction dLambda="5" DiffOrder="2" WEP="0.05" airPLS\_P="0.05"

Manual\_Region\_Selection: [172.717 - 1600 Raman Shift (cm-1)]

PLS1R MaxFacNum="19" Regression\_Algorithm="PLS\_Improved\_Kernel"

Validation\_method="Cross\_Validation" Cross\_Validation\_Method="Random" nFold="21"

No. of Factors: 7

Q-Residual Limit (0.01): 1428.42

MD Limit (0.01): 6.69447

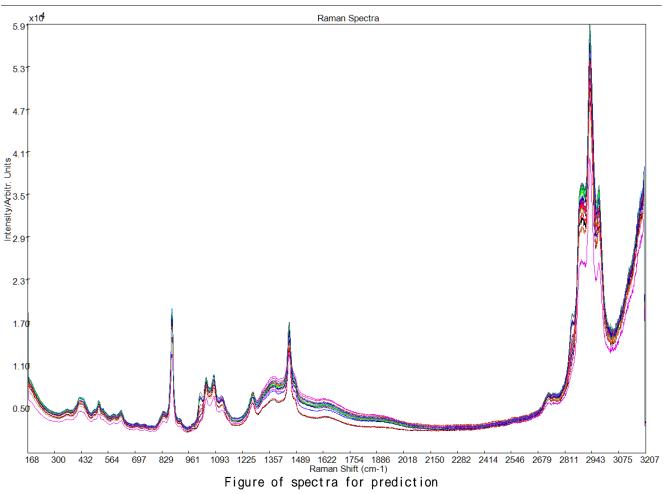
BWIQ Version (Current): 4.1.2
BWIQ Version (Model): 4.1.2

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Model creation time: 2019-08-12 11:04:47

## Prediction Results:

Title	Y1
1_4_0.33%MeOH.txt	0.3201
1_5_0.33%MeOH.txt	0.3451
2_4_0.66%MeOH.txt	0.6181
2_5_0.66%MeOH.txt	0.8391
3_4_0.99%MeOH.txt	1.0219
3_5_0.99%MeOH.txt	1.0008
4_4_1.64%MeOH.txt	1.7824
4_5_1.64%MeOH.txt	1.8099
5_4_2.28%MeOH.txt	2.2163
5_5_2.28%MeOH.txt	2.2184
6_4_2.91%MeOH.txt	2.5386
6_5_2.91%MeOH.txt	2.8046
7_4_4.15%MeOH.txt	4.2497
7_5_4.15%MeOH.txt	4.3005
8_4_4.76%MeOH.txt	4.8417
9_4_5.36%MeOH.txt	5.2567
9_5_5.36%MeOH.txt	5.4361



User Signature/Date